

Supporting Information

Post-Protein Binding Metal-Mediated Coupling of an Acridine Orange-Based Fluorophore.

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Table S2. XYZ coordinates of QM/MM optimized structure of **Lys2**.

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Figure S1. QM/MM optimized structure of **Lys1**.

Figure S2. QM/MM optimized structure of **Lys2**.

Figure S3. Dynamic light scattering (DLS) of an aqueous solution of (from top to bottom) **Lys**, **Lys1** and **Lys2**.

Figure S4. Circular dichroism (CD) spectra of **Lys**, **Lys1** and **Lys2**. Samples were recorded in a 50mM ammonium acetate buffer (pH 4.6) in 0.9M NaCl.

Figure S5. Intrinsic fluorescence spectra of **Lys**, **Lys1** and **Lys2**.

Table S1. XYZ coordinates of QM/MM optimized structure of **Lys1**.

TITLE	Lys1					HETATM	84	O	0	-8.005	-4.506	5.907	O
REMARK	1 File created by GaussView 5.0.9					HETATM	85	C	0	-7.974	-3.514	2.732	C
HETATM	1	N	0	-0.779 -11.588 -7.908	N	HETATM	86	C	0	-6.820	-3.444	1.756	C
HETATM	2	C	0	-2.241 -11.602 -7.839	C	HETATM	87	S	0	-6.915	-2.002	0.712	S
HETATM	3	C	0	-2.783 -10.244 -8.216	C	HETATM	88	C	0	-5.213	-1.903	0.111	C
HETATM	4	O	0	-2.305 -9.242 -7.632	O	HETATM	89	N	0	-9.978	-4.851	4.848	N
HETATM	5	C	0	-2.707 -11.990 -6.425	C	HETATM	90	C	0	-10.756	-4.784	6.076	C
HETATM	6	C	0	-4.242 -12.045 -6.305	C	HETATM	91	C	0	-10.414	-5.941	7.015	C
HETATM	7	C	0	-4.660 -12.730 -5.001	C	HETATM	92	O	0	-10.201	-5.716	8.212	O
HETATM	8	C	0	-6.175 -12.705 -4.802	C	HETATM	93	C	0	-12.252	-4.779	5.774	C
HETATM	9	N	0	-6.514 -13.398 -3.563	N	HETATM	94	C	0	-13.091	-4.645	7.034	C
HETATM	10	N	0	-3.732 -10.176 -9.157	N	HETATM	95	C	0	-14.559	-4.474	6.687	C
HETATM	11	C	0	-4.492 -8.964 -9.435	C	HETATM	96	C	0	-15.365	-4.300	7.971	C
HETATM	12	C	0	-5.834 -9.055 -8.746	C	HETATM	97	N	0	-16.784	-3.916	7.676	N
HETATM	13	O	0	-6.684 -9.886 -9.152	O	HETATM	98	N	0	-10.303	-7.149	6.452	N
HETATM	14	C	0	-4.632 -8.646 -10.977	C	HETATM	99	C	0	-8.651	-8.139	7.936	C
HETATM	15	C	0	-5.441 -7.374 -11.226	C	HETATM	100	O	0	-8.485	-8.524	9.082	O
HETATM	16	C	0	-3.243 -8.532 -11.661	C	HETATM	101	C	0	-9.647	-10.895	7.096	C
HETATM	17	N	0	-6.012 -8.246 -7.693	N	HETATM	102	C	0	-10.685	-11.254	8.166	C
HETATM	18	C	0	-7.310 -8.155 -6.985	C	HETATM	103	N	0	-10.415	-12.602	8.687	N
HETATM	19	C	0	-8.352 -7.427 -7.781	C	HETATM	104	C	0	-11.454	-13.037	9.641	C
HETATM	20	O	0	-8.061 -6.478 -8.520	O	HETATM	105	N	0	-12.557	-13.660	8.907	N
HETATM	21	C	0	-7.179 -7.423 -5.646	C	HETATM	106	N	0	-10.886	-14.016	10.573	N
HETATM	22	C	0	-6.612 -8.266 -4.558	C	HETATM	107	N	0	-7.717	-7.477	7.244	N
HETATM	23	C	0	-7.460 -8.885 -3.631	C	HETATM	108	C	0	-6.360	-7.237	7.768	C
HETATM	24	C	0	-5.220 -8.500 -4.470	C	HETATM	109	C	0	-6.200	-5.921	8.555	C
HETATM	25	C	0	-6.954 -9.693 -2.593	C	HETATM	110	O	0	-5.082	-5.502	8.908	O
HETATM	26	C	0	-4.706 -9.313 -3.457	C	HETATM	111	C	0	-5.333	-7.396	6.627	C
HETATM	27	C	0	-5.560 -9.914 -2.513	C	HETATM	112	C	0	-5.208	-8.878	6.287	C
HETATM	28	N	0	-9.607 -7.853 -7.602	N	HETATM	113	N	0	-4.318	-9.687	7.011	N
HETATM	29	C	0	-10.719 -6.987 -7.943	C	HETATM	114	C	0	-5.905	-9.767	5.480	C
HETATM	30	C	0	-10.873 -5.949 -6.843	C	HETATM	115	C	0	-4.504	-10.994	6.661	C
HETATM	31	O	0	-10.398 -6.137 -5.730	O	HETATM	116	N	0	-5.471	-11.086	5.726	N
HETATM	32	N	0	-11.516 -4.840 -7.178	N	HETATM	117	N	0	-7.314	-5.266	8.857	N
HETATM	33	C	0	-11.726 -3.730 -6.263	C	HETATM	118	C	0	-7.324	-4.148	9.815	C
HETATM	34	C	0	-12.400 -4.119 -4.921	C	HETATM	119	C	0	-6.982	-2.749	9.332	C
HETATM	35	O	0	-11.874 -3.821 -3.832	O	HETATM	120	O	0	-6.631	-1.874	10.139	O
HETATM	36	C	0	-12.499 -2.665 -7.033	C	HETATM	121	N	0	-7.091	-2.519	8.027	N
HETATM	37	C	0	-12.935 -1.497 -6.241	C	HETATM	122	C	0	-6.818	-1.188	7.468	C
HETATM	38	C	0	-13.734 -0.511 -7.152	C	HETATM	123	C	0	-7.993 -0.216	7.499	C	
HETATM	39	N	0	-15.023 -1.051 -7.605	N	HETATM	124	O	0	-7.822	0.994	7.359	O
HETATM	40	C	0	-16.160 -1.034 -6.898	C	HETATM	125	C	0	-6.340	-1.301	6.015	C
HETATM	41	N	0	-16.225 -0.487 -5.684	N	HETATM	126	C	0	-4.850	-1.524	5.798	C
HETATM	42	N	0	-17.261 -1.548 -7.430	N	HETATM	127	C	0	-4.559	-1.421	4.292	C
HETATM	43	N	0	-13.558 -4.799 -4.981	N	HETATM	128	C	0	-3.926	-0.544	6.621	C
HETATM	44	C	0	-14.256 -5.177 -3.747	C	HETATM	129	N	0	-9.198	-0.756	7.654	N
HETATM	45	C	0	-13.513 -6.292 -3.001	C	HETATM	130	C	0	-10.399	0.054	7.640	C
HETATM	46	O	0	-13.518 -6.323 -1.779	O	HETATM	131	C	0	-10.365	1.048	8.813	C
HETATM	47	C	0	-15.717 -5.587 -4.014	C	HETATM	132	O	0	-10.390	0.659	9.993	O
HETATM	48	S	0	-16.755 -4.227 -4.562	S	HETATM	133	C	0	-11.637	-0.853	7.672	C
HETATM	49	N	0	-12.886 -7.198 -3.758	N	HETATM	134	C	0	-12.927	-0.087	7.498	C
HETATM	50	C	0	-12.072 -8.258 -3.203	C	HETATM	135	O	0	-12.868	1.137	7.196	O
HETATM	51	C	0	-10.920 -7.669 -2.363	C	HETATM	136	O	0	-14.038	-0.743	7.656	O
HETATM	52	O	0	-10.682 -8.081 -1.217	O	HETATM	137	N	0	-10.247	2.325	8.461	N
HETATM	53	C	0	-11.535 -9.149 -4.330	C	HETATM	138	C	0	-9.983	3.420	9.400	C
HETATM	54	C	0	-10.715 -10.282 -3.794	C	HETATM	139	C	0	-8.712	3.443	10.219	C
HETATM	55	C	0	-10.022 -11.154 -4.836	C	HETATM	140	O	0	-8.633	4.172	11.224	O
HETATM	56	O	0	-9.828 -10.735 -6.125	O	HETATM	141	C	0	-11.181	3.694	10.291	C
HETATM	57	O	0	-9.636 -12.264 -4.357	O	HETATM	142	C	0	-12.035	4.765	9.714	C
HETATM	58	N	0	-10.250 -6.657 -2.900	N	HETATM	143	O	0	-11.651	5.959	9.701	O
HETATM	59	C	0	-9.184 -6.013 -2.104	C	HETATM	144	N	0	-13.168	4.356	9.149	N
HETATM	60	C	0	-9.711 -5.214 -0.917	C	HETATM	145	N	0	-7.729	2.634	9.807	N
HETATM	61	O	0	-9.098 -5.215 0.157	O	HETATM	146	C	0	-6.424	2.666	10.424	C
HETATM	62	C	0	-8.291 -5.112 -2.990	C	HETATM	147	C	0	-5.861	4.076	10.332	C
HETATM	63	C	0	-7.113 -4.445 -2.278	C	HETATM	148	O	0	-5.834	4.715	9.242	O
HETATM	64	C	0	-6.162 -5.486 -1.657	C	HETATM	149	C	0	-5.455	1.644	9.778	C
HETATM	65	C	0	-6.411 -3.504 -3.289	C	HETATM	150	C	0	-4.201	1.475	10.606	C
HETATM	66	N	0	-10.839 -4.532 -1.101	N	HETATM	151	C	0	-4.156	0.542	11.658	C
HETATM	67	C	0	-11.463 -3.798 0.000	C	HETATM	152	C	0	-3.093	2.287	10.406	C
HETATM	68	C	0	-11.750 -4.750 1.163	C	HETATM	153	C	0	-3.004	0.412	12.465	C
HETATM	69	O	0	-11.426 -4.457 2.323	O	HETATM	154	C	0	-1.938	2.157	11.203	C
HETATM	70	C	0	-12.748 -3.077 -0.472	C	HETATM	155	C	0	-1.916	1.232	12.245	C
HETATM	71	N	0	-12.313 -5.908 0.830	N	HETATM	156	O	0	-0.768	1.071	13.018	O
HETATM	72	C	0	-12.625 -6.929 1.823	C	HETATM	157	N	0	-5.426	4.602	11.488	N
HETATM	73	C	0	-11.376 -7.424 2.533	C	HETATM	158	C	0	-5.932	6.994	10.943	C
HETATM	74	O	0	-11.332 -7.485 3.768	O	HETATM	159	O	0	-5.535	8.034	10.423	O
HETATM	75	C	0	-13.365 -8.067 1.165	C	HETATM	160	C	0	-2.080	6.827	12.833	C
HETATM	76	N	0	-10.366 -7.785 1.755	N	HETATM	161	N	0	-0.946	6.596	13.742	N
HETATM	77	C	0	-9.112 -8.259 2.322	C	HETATM	162	C	0	-0.762	5.528	14.530	C
HETATM	78	C	0	-8.480 -7.184 3.204	C	HETATM	163	N	0	-2.061	5.061	15.036	N
HETATM	79	O	0	-7.958 -7.493 4.271	O	HETATM	164	N	0	0.100	5.898	15.662	N
HETATM	80	C	0	-8.170 -8.698 1.233	C	HETATM	165	N	0	-7.224	6.664	11.011	N
HETATM	81	N	0	-8.493 -5.929 2.737	N	HETATM	166	C	0	-8.269	7.581	10.563	C
HETATM	82	C	0	-7.952 -4.832 3.525	C	HETATM	167	C	0	-8.549	7.569	9.066	C
HETATM	83	C	0	-8.652 -4.699 4.866	C	HETATM	168	O	0	-9.366	8.356	8.575	O

HETATM 169 N	0	-7.863	6.681	8.331	N	HETATM 257 C	0	-3.444	5.601	-8.257	C
HETATM 170 C	0	-8.071	6.626	6.890	C	HETATM 258 C	0	-4.794	5.968	-8.817	C
HETATM 171 C	0	-9.087	5.570	6.512	C	HETATM 259 C	0	-5.750	6.557	-8.018	C
HETATM 172 O	0	-8.882	4.385	6.790	O	HETATM 260 C	0	-5.118	5.646	-10.156	C
HETATM 173 C	0	-6.734	6.360	6.197	C	HETATM 261 C	0	-7.001	6.894	-8.530	C
HETATM 174 C	0	-5.861	7.585	6.254	C	HETATM 262 C	0	-6.402	5.951	-10.674	C
HETATM 175 C	0	-5.950	8.573	5.255	C	HETATM 263 C	0	-7.332	6.582	-9.834	C
HETATM 176 C	0	-4.930	7.753	7.310	C	HETATM 264 N	0	-1.330	3.091	-7.194	N
HETATM 177 C	0	-5.103	9.706	5.284	C	HETATM 265 C	0	0.041	2.669	-6.986	C
HETATM 178 C	0	-4.085	8.880	7.349	C	HETATM 266 C	0	0.386	1.441	-7.835	C
HETATM 179 C	0	-4.182	9.847	6.322	C	HETATM 267 O	0	1.479	1.342	-8.396	O
HETATM 180 O	0	-3.387	10.994	6.307	O	HETATM 268 C	0	0.287	2.335	-5.507	C
HETATM 181 N	0	-10.216	6.018	5.938	N	HETATM 269 C	0	0.391	3.563	-4.578	C
HETATM 182 C	0	-11.289	5.059	5.575	C	HETATM 270 C	0	1.541	4.551	-4.916	C
HETATM 183 C	0	-10.809	4.066	4.522	C	HETATM 271 O	0	2.436	4.205	-5.743	O
HETATM 184 O	0	-9.884	4.379	3.757	O	HETATM 272 O	0	1.525	5.730	-4.322	O
HETATM 185 C	0	-12.523	5.785	5.061	C	HETATM 273 N	0	-0.529	0.456	-7.873	N
HETATM 186 O	0	-12.209	6.529	3.891	O	HETATM 274 C	0	-0.211	-0.880	-8.465	C
HETATM 187 N	0	-11.456	2.894	4.473	N	HETATM 275 C	0	-1.264	-1.458	-9.394	C
HETATM 188 C	0	-11.142	1.883	3.466	C	HETATM 276 O	0	-1.091	-2.575	-9.934	O
HETATM 189 C	0	-10.990	2.406	2.050	C	HETATM 277 C	0	-0.025	-1.901	-7.346	C
HETATM 190 O	0	-10.090	1.973	1.334	O	HETATM 278 O	0	-1.267	-2.121	-6.683	O
HETATM 191 C	0	-12.220	0.796	3.398	C	HETATM 279 N	0	-2.369	-0.710	-9.573	N
HETATM 192 C	0	-12.004	-0.672	3.755	C	HETATM 280 C	0	-3.542	-1.233	-10.302	C
HETATM 193 C	0	-13.158	-1.524	3.156	C	HETATM 281 C	0	-4.016	-2.553	-9.689	C
HETATM 194 C	0	-10.591	-1.223	3.454	C	HETATM 282 O	0	-4.435	-3.471	-10.408	O
HETATM 195 N	0	-11.895	3.270	1.617	N	HETATM 283 C	0	-3.291	-1.387	-11.801	C
HETATM 196 C	0	-11.811	3.873	0.283	C	HETATM 284 C	0	-4.565	-1.300	-12.605	C
HETATM 197 C	0	-10.464	4.555	-0.010	C	HETATM 285 O	0	-5.605	-0.829	-12.117	O
HETATM 198 O	0	-9.976	4.490	-1.134	O	HETATM 286 N	0	-4.502	-1.778	-13.842	N
HETATM 199 N	0	-9.851	5.180	0.991	N	HETATM 287 N	0	-3.874	-2.647	-8.380	N
HETATM 200 C	0	-8.508	5.759	0.825	C	HETATM 288 C	0	-4.310	-3.805	-7.592	C
HETATM 201 C	0	-7.445	4.749	0.443	C	HETATM 289 C	0	-3.483	-5.091	-7.826	C
HETATM 202 O	0	-6.628	4.991	-0.441	O	HETATM 290 O	0	-3.897	-6.216	-7.441	O
HETATM 203 C	0	-8.068	6.543	2.077	C	HETATM 291 C	0	-5.806	-4.098	-7.874	C
HETATM 204 C	0	-8.747	7.910	2.160	C	HETATM 292 C	0	-6.755	-2.984	-7.569	C
HETATM 205 O	0	-8.361	8.853	1.431	O	HETATM 293 C	0	-6.615	-2.171	-6.438	C
HETATM 206 N	0	-9.798	8.017	3.009	N	HETATM 294 C	0	-7.892	-2.831	-8.366	C
HETATM 207 N	0	-7.503	3.606	1.112	N	HETATM 295 C	0	-7.562	-1.186	-6.139	C
HETATM 208 C	0	-6.549	2.526	0.929	C	HETATM 296 C	0	-8.849	-1.896	-8.069	C
HETATM 209 C	0	-6.759	1.864	-0.402	C	HETATM 297 C	0	-8.680	-1.031	-6.968	C
HETATM 210 O	0	-5.791	1.514	-1.066	O	HETATM 298 N	0	-2.290	-4.924	-8.393	N
HETATM 211 C	0	-6.706	1.499	2.080	C	HETATM 299 C	0	-1.395	-6.044	-8.722	C
HETATM 212 C	0	-6.290	2.084	3.411	C	HETATM 300 C	0	-0.335	-6.243	-7.635	C
HETATM 213 C	0	-7.105	2.532	4.434	C	HETATM 301 O	0	0.547	-5.386	-7.458	O
HETATM 214 C	0	-4.938	2.362	3.835	C	HETATM 302 C	0	-0.756	-5.777	-10.072	C
HETATM 215 N	0	-6.331	3.048	5.461	N	HETATM 303 C	0	0.087	-6.923	-10.585	C
HETATM 216 C	0	-5.008	2.961	5.120	C	HETATM 304 O	0	0.288	-7.930	-9.901	O
HETATM 217 C	0	-3.674	2.135	3.255	C	HETATM 305 N	0	0.523	-6.799	-11.833	N
HETATM 218 C	0	-3.853	3.310	5.855	C	HETATM 306 N	0	-0.440	-7.334	-6.887	N
HETATM 219 C	0	-2.530	2.526	3.969	C	HETATM 307 C	0	0.513	-7.565	-5.809	C
HETATM 220 C	0	-2.632	3.113	5.242	C	HETATM 308 C	0	1.943	-7.684	-6.307	C
HETATM 221 N	0	-8.027	1.658	-0.784	N	HETATM 309 O	0	2.850	-7.428	-5.539	O
HETATM 222 C	0	-8.334	1.080	-2.101	C	HETATM 310 C	0	0.206	-8.830	-4.949	C
HETATM 223 C	0	-7.919	1.994	-3.264	C	HETATM 311 O	0	0.404	-10.012	-5.758	O
HETATM 224 O	0	-7.317	1.524	-4.238	O	HETATM 312 C	0	-1.217	-8.758	-4.394	C
HETATM 225 C	0	-9.836	0.612	-2.216	C	HETATM 313 N	0	2.149	-8.035	-7.568	N
HETATM 226 C	0	-10.172	0.092	-3.627	C	HETATM 314 C	0	3.502	-8.280	-8.054	C
HETATM 227 C	0	-10.111	-0.476	-1.162	C	HETATM 315 C	0	4.186	-7.032	-8.642	C
HETATM 228 N	0	-8.215	3.279	-3.127	N	HETATM 316 O	0	5.331	-7.148	-9.094	O
HETATM 229 C	0	-7.795	4.308	-4.078	C	HETATM 317 C	0	3.524	-9.410	-9.097	C
HETATM 230 C	0	-6.252	4.331	-4.203	C	HETATM 318 C	0	3.051	-10.773	-8.517	C
HETATM 231 O	0	-5.734	4.302	-5.305	O	HETATM 319 C	0	3.378	-11.881	-9.452	C
HETATM 232 C	0	-8.341	5.683	-3.644	C	HETATM 320 O	0	2.522	-12.324	-10.239	O
HETATM 233 S	0	-7.996	6.892	-4.879	S	HETATM 321 N	0	4.634	-12.293	-9.456	N
HETATM 234 N	0	-5.549	4.316	-3.070	N	HETATM 322 N	0	3.522	-5.867	-8.606	N
HETATM 235 C	0	-4.075	4.297	-3.128	C	HETATM 323 C	0	4.044	-4.622	-9.227	C
HETATM 236 C	0	-3.585	3.065	-3.846	C	HETATM 324 C	0	5.381	-4.235	-8.577	C
HETATM 237 O	0	-2.674	3.132	-4.677	O	HETATM 325 O	0	5.491	-4.171	-7.346	O
HETATM 238 C	0	-3.452	4.401	-1.737	C	HETATM 326 C	0	3.042	-3.470	-9.016	C
HETATM 239 N	0	-4.151	1.898	-3.529	N	HETATM 327 N	0	6.355	-3.936	-9.415	N
HETATM 240 C	0	-3.693	0.679	-4.197	C	HETATM 328 C	0	7.631	-3.380	-8.964	C
HETATM 241 C	0	-3.973	0.712	-5.711	C	HETATM 329 C	0	7.961	-2.210	-9.882	C
HETATM 242 O	0	-3.166	0.241	-6.514	O	HETATM 330 O	0	7.708	-2.260	-11.099	O
HETATM 243 C	0	-4.353	-0.523	-3.570	C	HETATM 331 C	0	8.803	-4.427	-9.014	C
HETATM 244 N	0	-5.141	1.240	-6.103	N	HETATM 332 O	0	9.015	-4.881	-10.355	O
HETATM 245 C	0	-5.471	1.329	-7.521	C	HETATM 333 C	0	8.528	-5.647	-8.112	C
HETATM 246 C	0	-4.399	2.117	-8.300	C	HETATM 334 N	0	8.542	-1.144	-9.326	N
HETATM 247 O	0	-3.881	1.634	-9.336	O	HETATM 335 C	0	8.936	-0.013	-10.154	C
HETATM 248 C	0	-6.833	2.028	-7.660	C	HETATM 336 C	0	10.208	0.594	-9.579	C
HETATM 249 C	0	-7.210	2.425	-9.047	C	HETATM 337 O	0	10.244	0.909	-8.391	O
HETATM 250 C	0	-7.544	1.208	-9.919	C	HETATM 338 C	0	7.822	1.051	-10.209	C
HETATM 251 C	0	-7.770	1.652	-11.358	C	HETATM 339 C	0	6.652	0.620	-11.084	C
HETATM 252 N	0	-8.041	0.439	-12.185	N	HETATM 340 O	0	6.777	0.506	-12.328	O
HETATM 253 N	0	-4.018	3.275	-7.769	N	HETATM 341 N	0	5.513	0.355	-10.444	N
HETATM 254 C	0	-3.102	4.137	-8.510	C	HETATM 342 N	0	11.226	0.760	-10.436	N
HETATM 255 C	0	-1.625	3.808	-8.269	C	HETATM 343 C	0	12.521	1.374	-10.034	C
HETATM 256 O	0	-0.774	4.181	-9.070	O	HETATM 344 C	0	12.399	2.887	-9.946	C

HETATM 345	O	0	11.871	3.546	-10.880	O	HETATM 433	N	0	3.226	-0.234	-3.289	N
HETATM 346	C	0	13.614	1.036	-11.040	C	HETATM 434	C	0	4.466	0.379	-3.800	C
HETATM 347	C	0	15.052	1.203	-10.479	C	HETATM 435	C	0	5.387	0.901	-2.687	C
HETATM 348	C	0	15.418	-0.018	-9.689	C	HETATM 436	O	0	5.863	2.051	-2.712	O
HETATM 349	N	0	16.712	0.086	-9.002	N	HETATM 437	C	0	4.133	1.458	-4.825	C
HETATM 350	C	0	17.838	-0.523	-9.380	C	HETATM 438	C	0	3.606	0.817	-6.108	C
HETATM 351	N	0	17.891	-1.287	-10.474	N	HETATM 439	C	0	4.693	0.017	-6.821	C
HETATM 352	N	0	18.927	-0.387	-8.641	N	HETATM 440	O	0	5.550	0.608	-7.499	O
HETATM 353	N	0	12.907	3.440	-8.847	N	HETATM 441	N	0	4.649	-1.314	-6.709	N
HETATM 354	C	0	12.995	4.880	-8.637	C	HETATM 442	N	0	5.659	0.005	-1.756	N
HETATM 355	C	0	14.306	5.443	-9.180	C	HETATM 443	C	0	6.493	0.331	-0.592	C
HETATM 356	O	0	15.287	4.722	-9.314	O	HETATM 444	C	0	7.957	0.342	-0.993	C
HETATM 357	C	0	12.868	5.192	-7.134	C	HETATM 445	O	0	8.421	-0.585	-1.661	O
HETATM 358	C	0	11.586	4.663	-6.534	C	HETATM 446	C	0	6.157	-0.657	0.524	C
HETATM 359	O	0	11.581	4.019	-5.464	O	HETATM 447	C	0	4.712	-0.348	1.045	C
HETATM 360	N	0	10.489	4.877	-7.245	N	HETATM 448	C	0	7.192	-0.615	1.659	C
HETATM 361	N	0	14.304	6.733	-9.508	N	HETATM 449	C	0	4.214	-1.418	2.058	C
HETATM 362	C	0	15.499	7.394	-10.062	C	HETATM 450	N	0	8.654	1.419	-0.598	N
HETATM 363	C	0	16.730	7.299	-9.153	C	HETATM 451	C	0	9.980	1.812	-1.104	C
HETATM 364	O	0	17.867	7.206	-9.634	O	HETATM 452	C	0	11.140	1.153	-0.331	C
HETATM 365	C	0	15.214	8.865	-10.514	C	HETATM 453	O	0	11.166	1.232	0.916	O
HETATM 366	O	0	14.673	9.616	-9.421	O	HETATM 454	C	0	10.069	3.356	-1.049	C
HETATM 367	C	0	14.226	8.843	-11.658	C	HETATM 455	C	0	11.209	3.942	-1.886	C
HETATM 368	N	0	16.489	7.244	-7.851	N	HETATM 456	O	0	12.153	3.245	-2.235	O
HETATM 369	C	0	17.578	7.185	-6.881	C	HETATM 457	N	0	11.108	5.255	-2.223	N
HETATM 370	C	0	18.180	5.784	-6.700	C	HETATM 458	N	0	12.073	0.503	-1.040	N
HETATM 371	O	0	19.110	5.628	-5.904	O	HETATM 459	C	0	13.251	-0.112	-0.413	C
HETATM 372	C	0	17.133	7.785	-5.547	C	HETATM 460	C	0	14.184	0.933	0.242	C
HETATM 373	C	0	16.110	6.926	-4.807	C	HETATM 461	O	0	15.055	0.538	0.989	O
HETATM 374	O	0	15.728	5.829	-5.271	O	HETATM 462	C	0	14.065	-0.929	-1.430	C
HETATM 375	O	0	15.666	7.364	-3.667	O	HETATM 463	O	0	14.552	-0.047	-2.458	O
HETATM 376	N	0	17.619	4.781	-7.396	N	HETATM 464	N	0	13.999	2.218	-0.053	N
HETATM 377	C	0	18.094	3.409	-7.342	C	HETATM 465	C	0	14.804	3.338	0.514	C
HETATM 378	C	0	17.311	2.526	-6.370	C	HETATM 466	C	0	14.733	3.279	2.050	C
HETATM 379	O	0	17.495	1.314	-6.348	O	HETATM 467	O	0	15.736	3.494	2.745	O
HETATM 380	N	0	16.407	3.126	-5.592	N	HETATM 468	C	0	14.236	4.672	-0.003	C
HETATM 381	C	0	15.547	2.309	-4.738	C	HETATM 469	C	0	14.982	5.966	0.411	C
HETATM 382	C	0	14.481	1.698	-5.671	C	HETATM 470	C	0	15.973	6.373	-0.650	C
HETATM 383	O	0	14.367	2.091	-6.834	O	HETATM 471	N	0	17.303	5.889	-0.298	N
HETATM 384	C	0	14.904	3.130	-3.624	C	HETATM 472	C	0	18.235	5.466	-1.154	C
HETATM 385	O	0	14.061	4.141	-4.159	O	HETATM 473	N	0	18.017	5.425	-2.472	N
HETATM 386	N	0	13.718	0.748	-5.134	N	HETATM 474	N	0	19.397	5.047	-0.664	N
HETATM 387	C	0	12.575	0.143	-5.877	C	HETATM 475	N	0	13.554	2.952	2.571	N
HETATM 388	C	0	11.318	0.132	-5.015	C	HETATM 476	C	0	13.291	2.981	4.012	C
HETATM 389	O	0	11.401	-0.010	-3.795	O	HETATM 477	C	0	12.748	1.713	4.627	C
HETATM 390	C	0	12.973	-1.270	-6.323	C	HETATM 478	O	0	12.981	1.413	5.800	O
HETATM 391	O	0	14.176	-1.176	-7.103	O	HETATM 479	C	0	12.271	4.090	4.313	C
HETATM 392	C	0	11.899	-1.955	-7.192	C	HETATM 480	C	0	12.860	5.434	4.075	C
HETATM 393	N	0	10.144	0.299	-5.660	N	HETATM 481	C	0	12.572	6.285	3.051	C
HETATM 394	C	0	8.823	0.233	-4.986	C	HETATM 482	C	0	13.892	6.052	4.851	C
HETATM 395	C	0	8.196	-1.144	-5.247	C	HETATM 483	N	0	13.353	7.417	3.154	N
HETATM 396	O	0	8.251	-1.658	-6.381	O	HETATM 484	C	0	14.171	7.296	4.252	C
HETATM 397	C	0	7.874	1.351	-5.497	C	HETATM 485	C	0	14.614	5.665	6.001	C
HETATM 398	C	0	8.251	2.765	-4.993	C	HETATM 486	C	0	15.136	8.178	4.770	C
HETATM 399	O	0	9.181	2.913	-4.180	O	HETATM 487	C	0	15.581	6.545	6.524	C
HETATM 400	O	0	7.520	3.777	-5.423	O	HETATM 488	C	0	15.830	7.783	5.901	C
HETATM 401	N	0	7.686	-1.771	-4.183	N	HETATM 489	N	0	11.956	0.980	3.847	N
HETATM 402	C	0	7.156	-3.123	-4.253	C	HETATM 490	C	0	11.003	0.072	4.457	C
HETATM 403	C	0	5.692	-3.259	-3.857	C	HETATM 491	C	0	11.262	-1.410	4.337	C
HETATM 404	O	0	5.278	-2.739	-2.823	O	HETATM 492	O	0	10.824	-2.172	5.196	O
HETATM 405	C	0	7.978	-4.039	-3.326	C	HETATM 493	C	0	9.570	0.397	3.971	C
HETATM 406	C	0	9.416	-4.152	-3.749	C	HETATM 494	C	0	9.182	1.822	4.213	C
HETATM 407	C	0	9.845	-5.208	-4.574	C	HETATM 495	C	0	9.049	2.787	3.281	C
HETATM 408	C	0	10.361	-3.177	-3.362	C	HETATM 496	C	0	8.932	2.436	5.473	C
HETATM 409	C	0	11.187	-5.301	-4.986	C	HETATM 497	N	0	8.707	3.982	3.870	N
HETATM 410	C	0	11.700	-3.262	-3.759	C	HETATM 498	C	0	8.666	3.807	5.222	C
HETATM 411	C	0	12.094	-4.313	-4.558	C	HETATM 499	C	0	8.916	1.963	6.790	C
HETATM 412	O	0	13.397	-4.412	-4.953	O	HETATM 500	C	0	8.362	4.728	6.248	C
HETATM 413	N	0	4.941	-3.993	-4.678	N	HETATM 501	C	0	8.613	2.878	7.819	C
HETATM 414	C	0	3.634	-4.523	-4.224	C	HETATM 502	C	0	8.335	4.247	7.520	C
HETATM 415	C	0	2.448	-3.582	-4.381	C	HETATM 503	N	0	11.973	-1.835	3.304	N
HETATM 416	O	0	2.536	-2.516	-5.001	O	HETATM 504	C	0	12.204	-3.264	3.136	C
HETATM 417	N	0	1.318	-4.025	-3.846	N	HETATM 505	C	0	13.615	-3.442	2.604	C
HETATM 418	C	0	0.049	-3.306	-3.964	C	HETATM 506	O	0	14.204	-2.479	2.067	O
HETATM 419	C	0	0.086	-1.837	-3.535	C	HETATM 507	C	0	11.138	-3.922	2.231	C
HETATM 420	O	0	-0.582	-0.996	-4.140	O	HETATM 508	S	0	11.070	-3.260	0.516	S
HETATM 421	C	0	-1.168	-3.981	-3.231	C	HETATM 509	N	0	14.158	-4.648	2.772	N
HETATM 422	C	0	-0.869	-4.260	-1.749	C	HETATM 510	C	0	15.464	-4.947	2.212	C
HETATM 423	C	0	-1.736	-5.104	-4.083	C	HETATM 511	C	0	15.392	-5.675	0.876	C
HETATM 424	C	0	-2.172	-4.433	-0.906	C	HETATM 512	O	0	14.736	-6.728	0.790	O
HETATM 425	N	0	0.904	-1.530	-2.527	N	HETATM 513	C	0	16.299	-5.776	3.166	C
HETATM 426	C	0	1.081	-0.176	-2.098	C	HETATM 514	C	0	17.654	-6.090	2.556	C
HETATM 427	C	0	2.464	0.419	-2.400	C	HETATM 515	O	0	18.344	-5.176	2.105	O
HETATM 428	O	0	2.828	1.465	-1.856	O	HETATM 516	N	0	17.983	-7.347	2.444	N
HETATM 429	C	0	0.664	-0.010	-0.616	C	HETATM 517	N	0	16.014	-5.095	-0.153	N
HETATM 430	C	0	-0.862	-0.136	-0.351	C	HETATM 518	C	0	16.141	-5.780	-1.438	C
HETATM 431	C	0	-1.123	-0.351	1.169	C	HETATM 519	C	0	17.602	-6.057	-1.814	C
HETATM 432	C	0	-1.648	1.087	-0.913	C	HETATM 520	O	0	17.854	-6.603	-2.873	O

HETATM 521	C	0	15.367	-5.066	-2.565	C	HETATM 609	C	0	9.615	-7.636	5.387	C
HETATM 522	C	0	15.973	-3.715	-2.967	C	HETATM 610	C	0	9.368	-6.167	4.994	C
HETATM 523	O	0	17.056	-3.332	-2.474	O	HETATM 611	C	0	8.680	-8.208	6.477	C
HETATM 524	O	0	15.309	-2.995	-3.836	O	HETATM 612	C	0	7.992	-5.880	4.341	C
HETATM 525	N	0	18.531	-5.684	-0.936	N	HETATM 613	N	0	12.110	-8.856	3.758	N
HETATM 526	C	0	19.939	-6.016	-1.151	C	HETATM 614	C	0	12.608	-8.764	2.381	C
HETATM 527	C	0	20.661	-5.201	-2.211	C	HETATM 615	C	0	11.520	-8.129	1.517	C
HETATM 528	O	0	21.823	-5.504	-2.529	O	HETATM 616	O	0	10.323	-8.419	1.695	O
HETATM 529	N	0	19.982	-4.228	-2.801	N	HETATM 617	C	0	12.829	-10.224	1.952	C
HETATM 530	C	0	20.552	-3.389	-3.853	C	HETATM 618	C	0	12.101	-11.074	2.961	C
HETATM 531	C	0	20.203	-1.901	-3.735	C	HETATM 619	C	0	11.706	-10.226	4.141	C
HETATM 532	O	0	20.219	-1.155	-4.731	O	HETATM 620	N	0	11.920	-7.233	0.613	N
HETATM 533	C	0	20.185	-3.933	-5.261	C	HETATM 621	C	0	10.938	-6.576	-0.245	C
HETATM 534	C	0	18.700	-3.822	-5.585	C	HETATM 622	C	0	10.104	-7.612	-1.022	C
HETATM 535	C	0	18.495	-3.965	-7.081	C	HETATM 623	O	0	8.945	-7.361	-1.342	O
HETATM 536	N	0	17.193	-3.444	-7.466	N	HETATM 624	C	0	11.656	-5.619	-1.196	C
HETATM 537	C	0	16.580	-3.732	-8.618	C	HETATM 625	S	0	12.548	-4.272	-0.402	S
HETATM 538	N	0	17.144	-4.598	-9.451	N	HETATM 626	N	0	10.706	-8.744	-1.370	N
HETATM 539	N	0	15.378	-3.192	-8.931	N	HETATM 627	C	0	9.966	-9.838	-2.031	C
HETATM 540	N	0	19.867	-1.444	-2.535	N	HETATM 628	C	0	8.668	-10.231	-1.293	C
HETATM 541	C	0	19.619	-0.031	-2.337	C	HETATM 629	O	0	7.678	-10.627	-1.917	O
HETATM 542	C	0	20.566	0.537	-1.283	C	HETATM 630	C	0	10.877	-11.048	-2.315	C
HETATM 543	O	0	20.254	0.505	-0.085	O	HETATM 631	O	0	11.345	-11.636	-1.097	O
HETATM 544	C	0	18.145	0.238	-1.913	C	HETATM 632	N	0	8.669	-10.128	0.034	N
HETATM 545	O	0	17.289	-0.497	-2.809	O	HETATM 633	C	0	7.462	-10.421	0.838	C
HETATM 546	C	0	17.830	1.706	-1.971	C	HETATM 634	C	0	6.284	-9.543	0.479	C
HETATM 547	N	0	21.719	1.044	-1.728	N	HETATM 635	O	0	5.120	-9.932	0.701	O
HETATM 548	C	0	22.717	1.538	-0.767	C	HETATM 636	C	0	7.757	-10.282	2.319	C
HETATM 549	C	0	22.175	2.529	0.241	C	HETATM 637	N	0	6.587	-8.352	-0.038	N
HETATM 550	O	0	21.334	3.386	-0.090	O	HETATM 638	C	0	5.569	-7.389	-0.430	C
HETATM 551	C	0	23.756	2.191	-1.679	C	HETATM 639	C	0	4.909	-7.747	-1.775	C
HETATM 552	C	0	23.770	1.224	-2.916	C	HETATM 640	O	0	4.030	-7.015	-2.256	O
HETATM 553	C	0	22.263	0.966	-3.101	C	HETATM 641	C	0	6.186	-5.998	-0.475	C
HETATM 554	N	0	22.635	2.399	1.483	N	HETATM 642	C	0	6.792	-5.571	0.855	C
HETATM 555	C	0	22.424	3.439	2.488	C	HETATM 643	C	0	7.482	-4.222	0.628	C
HETATM 556	C	0	21.008	3.390	2.965	C	HETATM 644	C	0	5.663	-5.447	1.917	C
HETATM 557	O	0	20.532	4.308	3.629	O	HETATM 645	N	0	5.323	-8.865	-2.379	N
HETATM 558	N	0	20.361	2.282	2.618	N	HETATM 646	C	0	4.763	-9.240	-3.694	C
HETATM 559	C	0	18.957	2.034	2.782	C	HETATM 647	C	0	3.831	-10.439	-3.631	C
HETATM 560	C	0	18.642	1.550	4.193	C	HETATM 648	O	0	3.322	-10.879	-4.660	O
HETATM 561	O	0	19.479	0.931	4.856	O	HETATM 649	C	0	5.912	-9.549	-4.663	C
HETATM 562	C	0	18.565	0.942	1.780	C	HETATM 650	C	0	6.906	-8.404	-4.870	C
HETATM 563	O	0	17.291	0.449	2.030	O	HETATM 651	C	0	7.852	-8.834	-5.995	C
HETATM 564	N	0	17.421	1.822	4.648	N	HETATM 652	C	0	6.237	-7.073	-5.229	C
HETATM 565	C	0	16.919	1.124	5.826	C	HETATM 653	N	0	3.606	-10.942	-2.416	N
HETATM 566	C	0	15.892	0.047	5.451	C	HETATM 654	C	0	2.861	-12.190	-2.208	C
HETATM 567	O	0	15.476	-0.067	4.266	O	HETATM 655	C	0	1.385	-11.993	-2.476	C
HETATM 568	C	0	16.299	2.110	6.825	C	HETATM 656	O	0	0.836	-10.895	-2.183	O
HETATM 569	C	0	17.234	3.265	7.196	C	HETATM 657	C	0	3.091	-12.711	-0.782	C
HETATM 570	C	0	18.350	2.796	8.161	C	HETATM 658	O	0	2.504	-13.974	-0.626	O
HETATM 571	N	0	17.820	2.537	9.501	N	HETATM 659	N	0	0.643	-13.029	-2.953	N
HETATM 572	C	0	17.658	3.465	10.449	C	HETATM 660	C	0	-0.820	-12.983	-3.118	C
HETATM 573	N	0	18.016	4.726	10.229	N	HETATM 661	C	0	-1.515	-12.733	-1.803	C
HETATM 574	N	0	17.149	3.134	11.633	N	HETATM 662	O	0	-2.609	-12.104	-1.785	O
HETATM 575	N	0	15.513	-0.727	6.470	N	HETATM 663	C	0	-1.329	-14.293	-3.745	C
HETATM 576	C	0	14.601	-1.865	6.372	C	HETATM 664	O	0	-0.973	-15.406	-2.966	O
HETATM 577	C	0	13.710	-1.843	7.612	C	HETATM 665	N	0	-0.990	-13.312	-0.601	N
HETATM 578	O	0	13.713	-2.796	8.426	O	HETATM 666	C	0	-1.365	-12.874	0.747	C
HETATM 579	C	0	15.409	-3.165	6.282	C	HETATM 667	C	0	-0.906	-11.448	0.971	C
HETATM 580	C	0	14.526	-4.451	6.264	C	HETATM 668	O	0	0.310	-11.168	0.787	O
HETATM 581	O	0	15.034	-5.570	6.392	O	HETATM 669	C	0	-0.722	-13.841	1.764	C
HETATM 582	N	0	13.230	-4.281	6.072	N	HETATM 670	C	0	-0.961	-13.453	3.191	C
HETATM 583	N	0	12.925	-0.771	7.706	N	HETATM 671	O	0	0.024	-13.256	3.949	O
HETATM 584	C	0	12.158	-0.421	8.905	C	HETATM 672	O	0	-2.248	-13.387	3.715	O
HETATM 585	C	0	10.969	-1.346	9.158	C	HETATM 673	N	0	-1.776	-10.486	1.402	N
HETATM 586	O	0	10.509	-1.470	10.291	O	HETATM 674	C	0	-1.379	-9.068	1.566	C
HETATM 587	C	0	11.708	1.032	8.815	C	HETATM 675	C	0	-0.885	-8.735	2.971	C
HETATM 588	C	0	12.437	2.180	9.540	C	HETATM 676	O	0	-0.622	-7.576	3.232	O
HETATM 589	C	0	13.779	1.769	10.142	C	HETATM 677	C	0	-2.535	-8.094	1.167	C
HETATM 590	C	0	12.558	3.394	8.674	C	HETATM 678	C	0	-3.724	-8.157	2.161	C
HETATM 591	N	0	10.502	-2.030	8.118	N	HETATM 679	C	0	-2.985	-8.374	-0.301	C
HETATM 592	C	0	9.486	-3.072	8.289	C	HETATM 680	C	0	-4.758	-7.082	1.976	C
HETATM 593	C	0	10.036	-4.463	8.591	C	HETATM 681	N	0	-0.767	-9.732	3.864	N
HETATM 594	O	0	9.259	-5.417	8.840	O	HETATM 682	C	0	-0.348	-9.455	5.265	C
HETATM 595	C	0	8.557	-3.099	7.061	C	HETATM 683	C	0	0.905	-8.556	5.394	C
HETATM 596	S	0	7.532	-1.620	7.008	S	HETATM 684	O	0	0.873	-7.552	6.087	O
HETATM 597	N	0	11.366	-4.585	8.576	N	HETATM 685	C	0	-0.198	-10.772	6.061	C
HETATM 598	C	0	12.082	-5.840	8.823	C	HETATM 686	O	0	-1.405	-11.488	5.992	O
HETATM 599	C	0	11.628	-7.019	7.987	C	HETATM 687	C	0	0.148	-10.521	7.533	C
HETATM 600	O	0	11.281	-8.063	8.506	O	HETATM 688	N	0	1.985	-8.930	4.713	N
HETATM 601	C	0	12.052	-6.195	10.328	C	HETATM 689	C	0	3.234	-8.166	4.794	C
HETATM 602	C	0	12.646	-5.089	11.171	C	HETATM 690	C	0	3.044	-6.716	4.344	C
HETATM 603	O	0	13.865	-4.870	11.135	O	HETATM 691	O	0	3.488	-5.778	5.028	O
HETATM 604	N	0	11.798	-4.355	11.900	N	HETATM 692	C	0	4.368	-8.877	4.002	C
HETATM 605	N	0	11.606	-6.834	6.668	N	HETATM 693	N	0	2.316	-6.516	3.242	N
HETATM 606	C	0	11.121	-7.852	5.760	C	HETATM 694	C	0	2.126	-5.169	2.715	C
HETATM 607	C	0	11.902	-7.722	4.458	C	HETATM 695	C	0	1.297	-4.344	3.694	C
HETATM 608	O	0	12.288	-6.593	4.082	O	HETATM 696	O	0	1.618	-3.198	3.973	O

HETATM 697	C	0	1.485	-5.177	1.327	C	HETATM 785	C	0	-0.225	10.007	7.114	C
HETATM 698	O	0	2.464	-5.549	0.362	O	HETATM 786	C	0	-0.059	9.384	5.730	C
HETATM 699	N	0	0.254	-4.965	4.234	N	HETATM 787	O	0	1.031	8.888	5.364	O
HETATM 700	C	0	-0.616	-4.280	5.190	C	HETATM 788	N	0	-1.109	9.465	4.929	N
HETATM 701	C	0	0.159	-3.899	6.448	C	HETATM 789	C	0	-1.050	8.803	3.606	C
HETATM 702	O	0	0.091	-2.732	6.893	O	HETATM 790	C	0	-0.296	9.609	2.534	C
HETATM 703	C	0	-1.881	-5.135	5.560	C	HETATM 791	O	0	-0.151	9.147	1.388	O
HETATM 704	C	0	-2.625	-4.477	6.732	C	HETATM 792	C	0	-2.444	8.385	3.128	C
HETATM 705	C	0	-2.792	-5.186	4.362	C	HETATM 793	C	0	-3.010	7.220	3.924	C
HETATM 706	N	0	0.895	-4.861	7.017	N	HETATM 794	S	0	-4.473	6.430	3.118	S
HETATM 707	C	0	1.616	-4.582	8.255	C	HETATM 795	C	0	-3.676	5.547	1.747	C
HETATM 708	C	0	2.622	-3.448	8.063	C	HETATM 796	N	0	0.210	10.786	2.911	N
HETATM 709	O	0	2.792	-2.598	8.955	O	HETATM 797	C	0	0.990	11.624	2.011	C
HETATM 710	C	0	2.338	-5.823	8.787	C	HETATM 798	C	0	2.312	10.939	1.651	C
HETATM 711	C	0	1.378	-6.882	9.278	C	HETATM 799	O	0	2.961	11.334	0.705	O
HETATM 712	O	0	0.175	-6.640	9.380	O	HETATM 800	C	0	1.248	13.002	2.625	C
HETATM 713	N	0	1.897	-8.078	9.539	N	HETATM 801	C	0	-0.020	13.828	2.753	C
HETATM 714	N	0	3.282	-3.453	6.895	N	HETATM 802	O	0	-0.644	14.203	1.746	O
HETATM 715	C	0	4.293	-2.438	6.650	C	HETATM 803	N	0	-0.373	14.182	3.998	N
HETATM 716	C	0	3.636	-1.067	6.388	C	HETATM 804	N	0	2.636	9.899	2.406	N
HETATM 717	O	0	4.098	-0.004	6.871	O	HETATM 805	C	0	3.745	9.006	2.086	C
HETATM 718	C	0	5.228	-2.906	5.512	C	HETATM 806	C	0	3.597	8.366	0.717	C
HETATM 719	S	0	6.608	-1.750	5.199	S	HETATM 807	O	0	4.602	7.999	0.102	O
HETATM 720	N	0	2.528	-1.086	5.639	N	HETATM 808	C	0	3.926	7.946	3.172	C
HETATM 721	C	0	1.769	0.144	5.398	C	HETATM 809	N	0	2.359	8.199	0.245	N
HETATM 722	C	0	1.238	0.796	6.696	C	HETATM 810	C	0	2.090	7.636	-1.094	C
HETATM 723	O	0	1.222	2.016	6.809	O	HETATM 811	C	0	1.787	8.780	-2.044	C
HETATM 724	C	0	0.637	-0.110	4.398	C	HETATM 812	O	0	0.699	9.389	-2.005	O
HETATM 725	N	0	0.879	-0.015	7.694	N	HETATM 813	C	0	0.936	6.617	-1.044	C
HETATM 726	C	0	0.508	0.538	9.017	C	HETATM 814	C	0	1.320	5.357	-0.333	C
HETATM 727	C	0	1.656	1.339	9.647	C	HETATM 815	C	0	2.005	4.288	-0.872	C
HETATM 728	O	0	1.434	2.383	10.249	O	HETATM 816	C	0	1.108	5.040	1.046	C
HETATM 729	C	0	0.068	-0.596	9.951	C	HETATM 817	N	0	2.191	3.305	0.089	N
HETATM 730	C	0	-1.298	-1.187	9.568	C	HETATM 818	C	0	1.685	3.762	1.278	C
HETATM 731	C	0	-1.648	-2.472	10.373	C	HETATM 819	C	0	0.512	5.725	2.129	C
HETATM 732	C	0	-3.038	-2.951	9.988	C	HETATM 820	C	0	1.633	3.125	2.514	C
HETATM 733	N	0	-3.487	-4.161	10.795	N	HETATM 821	C	0	0.473	5.071	3.395	C
HETATM 734	N	0	2.901	0.837	9.517	N	HETATM 822	C	0	1.028	3.792	3.565	C
HETATM 735	C	0	4.063	1.578	10.000	C	HETATM 823	N	0	2.741	9.099	-2.901	N
HETATM 736	C	0	4.308	2.883	9.227	C	HETATM 824	C	0	2.571	10.250	-3.773	C
HETATM 737	O	0	4.562	3.939	9.813	O	HETATM 825	C	0	1.309	10.132	-4.649	C
HETATM 738	C	0	5.325	0.724	9.909	C	HETATM 826	O	0	0.607	11.128	-4.797	O
HETATM 739	C	0	5.353	-0.404	10.854	C	HETATM 827	C	0	3.840	10.601	-4.592	C
HETATM 740	C	0	6.601	-1.290	10.606	C	HETATM 828	C	0	4.269	9.453	-5.467	C
HETATM 741	C	0	6.407	-2.631	11.336	C	HETATM 829	C	0	3.620	11.881	-5.437	C
HETATM 742	N	0	6.295	-2.347	12.810	N	HETATM 830	N	0	1.029	8.940	-5.176	N
HETATM 743	N	0	4.198	2.810	7.906	N	HETATM 831	C	0	-0.189	8.730	-5.973	C
HETATM 744	C	0	4.404	3.970	7.043	C	HETATM 832	C	0	-1.436	8.951	-5.119	C
HETATM 745	C	0	3.398	5.097	7.372	C	HETATM 833	O	0	-2.429	9.506	-5.627	O
HETATM 746	O	0	3.780	6.240	7.574	O	HETATM 834	C	0	-0.228	7.401	-6.653	C
HETATM 747	C	0	4.287	3.584	5.544	C	HETATM 835	N	0	-1.419	8.539	-3.841	N
HETATM 748	C	0	5.427	2.636	5.144	C	HETATM 836	C	0	-2.559	8.950	-2.984	C
HETATM 749	C	0	4.353	4.839	4.658	C	HETATM 837	C	0	-2.698	10.479	-2.868	C
HETATM 750	C	0	5.196	1.823	3.882	C	HETATM 838	O	0	-3.811	11.027	-3.020	O
HETATM 751	N	0	2.117	4.742	7.407	N	HETATM 839	C	0	-2.535	8.286	-1.587	C
HETATM 752	C	0	1.067	5.702	7.658	C	HETATM 840	C	0	-3.683	8.752	-0.705	C
HETATM 753	C	0	1.099	6.285	9.066	C	HETATM 841	C	0	-4.904	8.164	-0.601	C
HETATM 754	O	0	0.487	7.333	9.309	O	HETATM 842	C	0	-3.696	9.871	0.205	C
HETATM 755	C	0	-0.314	5.103	7.294	C	HETATM 843	N	0	-5.695	8.863	0.305	N
HETATM 756	C	0	-0.819	4.122	8.387	C	HETATM 844	C	0	-4.990	9.927	0.787	C
HETATM 757	C	0	-1.328	6.227	6.956	C	HETATM 845	C	0	-2.773	10.867	0.526	C
HETATM 758	N	0	1.834	5.610	9.964	N	HETATM 846	C	0	-5.362	10.907	1.744	C
HETATM 759	C	0	2.013	6.062	11.352	C	HETATM 847	C	0	-3.130	11.831	1.482	C
HETATM 760	C	0	3.206	6.968	11.549	C	HETATM 848	C	0	-4.427	11.861	2.051	C
HETATM 761	O	0	3.382	7.539	12.643	O	HETATM 849	N	0	-1.597	11.185	-2.614	N
HETATM 762	C	0	2.124	4.881	12.309	C	HETATM 850	C	0	-1.687	12.658	-2.493	C
HETATM 763	O	0	0.960	4.087	12.278	O	HETATM 851	C	0	-2.264	13.296	-3.764	C
HETATM 764	N	0	4.033	7.126	10.528	N	HETATM 852	O	0	-3.150	14.142	-3.679	O
HETATM 765	C	0	5.309	7.817	10.739	C	HETATM 853	C	0	-0.328	13.286	-2.143	C
HETATM 766	C	0	5.264	9.349	10.753	C	HETATM 854	C	0	-0.410	14.781	-1.820	C
HETATM 767	O	0	6.308	10.004	10.822	O	HETATM 855	C	0	0.943	15.384	-1.343	C
HETATM 768	C	0	6.399	7.276	9.818	C	HETATM 856	N	0	2.105	14.875	-2.081	N
HETATM 769	C	0	6.309	7.809	8.407	C	HETATM 857	C	0	2.512	15.310	-3.276	C
HETATM 770	O	0	5.527	8.825	8.137	O	HETATM 858	N	0	1.850	16.271	-3.916	N
HETATM 771	O	0	7.017	7.246	7.537	O	HETATM 859	N	0	3.583	14.766	-3.842	N
HETATM 772	N	0	4.064	9.932	10.710	N	HETATM 860	N	0	-1.790	12.830	-4.912	N
HETATM 773	C	0	3.942	11.395	10.835	C	HETATM 861	C	0	-2.072	13.479	-6.198	C
HETATM 774	C	0	3.238	12.126	9.701	C	HETATM 862	C	0	-3.364	13.007	-6.813	C
HETATM 775	O	0	2.550	13.118	9.945	O	HETATM 863	O	0	-3.941	13.714	-7.644	O
HETATM 776	N	0	3.347	11.625	8.469	N	HETATM 864	C	0	-0.911	13.238	-7.189	C
HETATM 777	C	0	2.732	12.326	7.344	C	HETATM 865	C	0	0.333	14.028	-6.832	C
HETATM 778	C	0	1.493	11.650	6.782	C	HETATM 866	O	0	0.234	15.114	-6.247	O
HETATM 779	O	0	0.999	12.039	5.721	O	HETATM 867	N	0	1.505	13.489	-7.177	N
HETATM 780	C	0	3.744	12.599	6.231	C	HETATM 868	N	0	-3.834	11.812	-6.440	N
HETATM 781	C	0	4.811	13.581	6.664	C	HETATM 869	C	0	-4.995	11.228	-7.137	C
HETATM 782	O	0	4.502	14.664	7.152	O	HETATM 870	C	0	-6.179	10.840	-6.257	C
HETATM 783	N	0	6.069	13.188	6.530	N	HETATM 871	O	0	-7.288	10.651	-6.757	O
HETATM 784	N	0	0.990	10.672	7.514	N	HETATM 872	C	0	-4.568	10.067	-8.055	C

HETATM 873	C	0	-3.412	10.500	-8.955	C	HETATM 961	C	0	-21.129	2.940	-4.651	C
HETATM 874	C	0	-2.819	9.352	-9.742	C	HETATM 962	C	0	-21.241	4.413	-5.077	C
HETATM 875	N	0	-3.774	8.938	-10.774	N	HETATM 963	N	0	-20.746	5.322	-4.029	N
HETATM 876	C	0	-3.495	8.020	-11.688	C	HETATM 964	C	0	-20.164	6.508	-4.246	C
HETATM 877	N	0	-2.299	7.454	-11.674	N	HETATM 965	N	0	-19.974	6.958	-5.481	N
HETATM 878	N	0	-4.395	7.691	-12.624	N	HETATM 966	N	0	-19.745	7.242	-3.213	N
HETATM 879	N	0	-5.962	10.733	-4.944	N	HETATM 967	N	0	-20.823	-0.503	-3.301	N
HETATM 880	C	0	-7.005	10.267	-4.033	C	HETATM 968	C	0	-21.391	-1.765	-3.729	C
HETATM 881	C	0	-7.421	11.299	-3.000	C	HETATM 969	C	0	-20.736	-3.014	-3.166	C
HETATM 882	O	0	-6.631	11.483	-2.738	O	HETATM 970	O	0	-21.241	-4.114	-3.362	O
HETATM 883	C	0	-6.536	9.006	-3.267	C	HETATM 971	N	0	-19.616	-2.865	-2.475	N
HETATM 884	S	0	-6.162	7.622	-4.374	S	HETATM 972	C	0	-18.906	-4.049	-2.001	C
HETATM 885	N	0	-6.423	11.923	-2.365	N	HETATM 973	C	0	-19.555	-4.677	-0.749	C
HETATM 886	C	0	-6.658	12.956	-1.358	C	HETATM 974	O	0	-19.847	-3.982	0.217	O
HETATM 887	C	0	-7.706	13.973	-1.815	C	HETATM 975	C	0	-17.453	-3.703	-1.688	C
HETATM 888	O	0	-7.585	14.540	-2.900	O	HETATM 976	S	0	-16.584	-2.891	-3.059	S
HETATM 889	C	0	-5.335	13.667	-1.063	C	HETATM 977	N	0	-19.725	-5.995	-0.775	N
HETATM 890	C	0	-5.373	14.646	0.104	C	HETATM 978	C	0	-20.078	-6.715	0.437	C
HETATM 891	C	0	-3.936	15.115	0.352	C	HETATM 979	C	0	-18.771	-6.892	1.184	C
HETATM 892	C	0	-3.839	16.068	1.548	C	HETATM 980	O	0	-17.868	-7.610	0.712	O
HETATM 893	N	0	-2.434	16.518	1.715	N	HETATM 981	C	0	-20.743	-8.058	0.117	C
HETATM 894	N	0	-8.733	14.179	-0.988	N	HETATM 982	C	0	-20.964	-8.960	1.343	C
HETATM 895	C	0	-9.769	15.183	-1.257	C	HETATM 983	C	0	-22.140	-9.936	1.200	C
HETATM 896	C	0	-10.896	14.697	-2.166	C	HETATM 984	N	0	-22.539	-10.277	-0.172	N
HETATM 897	O	0	-11.950	15.334	-2.254	O	HETATM 985	C	0	-21.768	-10.880	-1.085	C
HETATM 898	N	0	-10.699	13.564	-2.831	N	HETATM 986	N	0	-20.509	-11.193	-0.809	N
HETATM 899	C	0	-11.711	13.037	-3.747	C	HETATM 987	N	0	-22.256	-11.148	-2.295	N
HETATM 900	C	0	-12.785	12.211	-3.046	C	HETATM 988	N	0	-18.673	-6.233	2.335	N
HETATM 901	O	0	-12.698	11.924	-1.843	O	HETATM 989	C	0	-17.401	-6.074	3.069	C
HETATM 902	C	0	-11.044	12.201	-4.896	C	HETATM 990	C	0	-17.369	-6.856	4.385	C
HETATM 903	O	0	-10.641	10.915	-4.391	O	HETATM 991	O	0	-16.521	-7.738	4.557	O
HETATM 904	C	0	-9.885	12.943	-5.465	C	HETATM 992	C	0	-17.128	-4.605	3.371	C
HETATM 905	N	0	-13.798	11.801	-3.813	N	HETATM 993	C	0	-16.875	-3.665	2.200	C
HETATM 906	C	0	-14.838	10.932	-3.264	C	HETATM 994	C	0	-16.931	-2.226	2.692	C
HETATM 907	C	0	-14.309	9.498	-3.209	C	HETATM 995	C	0	-15.531	-3.984	1.559	C
HETATM 908	O	0	-14.638	8.668	-4.055	O	HETATM 996	O	0	-18.164	-6.603	5.296	O
HETATM 909	C	0	-16.116	11.035	-4.113	C	HETATM 997	Re	0	-6.254	-12.903	4.741	Re
HETATM 910	C	0	-17.263	10.144	-3.605	C	HETATM 998	C	0	-5.473	-12.434	3.061	C
HETATM 911	O	0	-17.209	9.608	-2.476	O	HETATM 999	O	0	-5.017	-12.107	2.019	O
HETATM 912	O	0	-18.311	9.985	-4.424	O	HETATM 1000	C	0	-7.001	-14.502	3.953	C
HETATM 913	N	0	-13.465	9.224	-2.208	N	HETATM 1001	O	0	-7.477	-15.469	3.463	O
HETATM 914	C	0	-12.836	7.890	-2.069	C	HETATM 1002	C	0	-7.805	-11.971	4.164	C
HETATM 915	C	0	-13.824	6.767	-1.700	C	HETATM 1003	O	0	-8.774	-11.413	3.773	O
HETATM 916	O	0	-13.561	5.606	-1.965	O	HETATM 1004	O	0	-4.421	-14.003	5.442	O
HETATM 917	C	0	-11.620	7.897	-1.098	C	HETATM 1005	O	0	-6.985	-13.386	6.796	O
HETATM 918	C	0	-10.528	8.848	-1.621	C	HETATM 1006	H	0	-2.310	-11.266	-5.684	H
HETATM 919	C	0	-12.057	8.293	0.306	C	HETATM 1007	H	0	-2.290	-12.992	-6.189	H
HETATM 920	N	0	-14.977	7.124	-1.133	N	HETATM 1008	H	0	-4.651	-11.010	-6.326	H
HETATM 921	C	0	-16.004	6.149	-0.803	C	HETATM 1009	H	0	-4.668	-12.610	-7.163	H
HETATM 922	C	0	-16.466	5.416	-2.071	C	HETATM 1010	H	0	-4.167	-12.226	-4.141	H
HETATM 923	O	0	-16.967	4.293	-1.985	O	HETATM 1011	H	0	-4.334	-13.791	-5.034	H
HETATM 924	C	0	-17.168	6.936	-0.206	C	HETATM 1012	H	0	-6.542	-11.655	-4.765	H
HETATM 925	C	0	-18.138	6.228	0.674	C	HETATM 1013	H	0	-6.668	-13.219	-5.656	H
HETATM 926	C	0	-19.145	7.254	1.173	C	HETATM 1014	H	0	-6.223	-12.797	-2.758	H
HETATM 927	O	0	-18.975	7.833	2.254	O	HETATM 1015	H	0	-7.553	-13.485	-3.510	H
HETATM 928	N	0	-20.151	7.562	0.335	N	HETATM 1016	H	0	-2.615	-12.380	-8.544	H
HETATM 929	N	0	-16.346	6.072	-3.235	N	HETATM 1017	H	0	-0.499	-11.377	-8.894	H
HETATM 930	C	0	-16.685	5.429	-4.523	C	HETATM 1018	H	0	-0.427	-12.553	-7.708	H
HETATM 931	C	0	-15.967	4.078	-4.740	C	HETATM 1019	H	0	-5.161	-9.468	-11.412	H
HETATM 932	O	0	-16.515	3.126	-5.328	O	HETATM 1020	H	0	-5.749	-6.958	-10.289	H
HETATM 933	C	0	-16.434	6.380	-5.714	C	HETATM 1021	H	0	-4.837	-6.663	-11.750	H
HETATM 934	N	0	-14.724	4.003	-4.243	N	HETATM 1022	H	0	-6.305	-7.609	-11.812	H
HETATM 935	C	0	-13.900	2.813	-4.377	C	HETATM 1023	H	0	-2.474	-8.695	-10.935	H
HETATM 936	C	0	-14.451	1.600	-3.642	C	HETATM 1024	H	0	-3.133	-7.556	-12.085	H
HETATM 937	O	0	-14.111	0.466	-3.969	O	HETATM 1025	H	0	-3.165	-9.267	-12.435	H
HETATM 938	C	0	-12.460	3.101	-3.909	C	HETATM 1026	H	0	-3.946	-8.134	-9.039	H
HETATM 939	C	0	-11.808	4.011	-4.896	C	HETATM 1027	H	0	-6.470	-6.638	-5.809	H
HETATM 940	C	0	-11.569	5.327	-4.758	C	HETATM 1028	H	0	-8.177	-7.186	-5.342	H
HETATM 941	C	0	-11.370	3.644	-6.208	C	HETATM 1029	H	0	-8.518	-8.742	-3.713	H
HETATM 942	N	0	-10.991	5.836	-5.906	N	HETATM 1030	H	0	-4.558	-8.053	-5.182	H
HETATM 943	C	0	-10.851	4.824	-6.816	C	HETATM 1031	H	0	-7.616	-10.133	-1.876	H
HETATM 944	C	0	-11.361	2.439	-6.927	C	HETATM 1032	H	0	-3.651	-9.481	-3.397	H
HETATM 945	C	0	-10.337	4.838	-8.098	C	HETATM 1033	H	0	-5.156	-10.533	-1.740	H
HETATM 946	C	0	-10.852	2.442	-8.224	C	HETATM 1034	H	0	-7.611	-9.170	-6.834	H
HETATM 947	C	0	-10.350	3.655	-8.800	C	HETATM 1035	H	0	-10.445	-6.461	-8.834	H
HETATM 948	N	0	-15.299	1.843	-2.642	N	HETATM 1036	H	0	-11.602	-7.591	-7.929	H
HETATM 949	C	0	-15.896	0.727	-1.931	C	HETATM 1037	H	0	-11.810	-2.279	-7.755	H
HETATM 950	C	0	-17.409	0.601	-2.207	C	HETATM 1038	H	0	-13.400	-3.143	-7.356	H
HETATM 951	O	0	-18.081	-0.227	-1.582	O	HETATM 1039	H	0	-12.048	-0.983	-5.935	H
HETATM 952	C	0	-15.580	0.745	-0.394	C	HETATM 1040	H	0	-13.622	-1.862	-5.507	H
HETATM 953	C	0	-16.253	1.924	0.326	C	HETATM 1041	H	0	-13.969	0.333	-6.536	H
HETATM 954	C	0	-14.042	0.625	-0.143	C	HETATM 1042	H	0	-13.143	-0.381	-8.034	H
HETATM 955	C	0	-16.209	1.826	1.888	C	HETATM 1043	H	0	-15.053	-1.465	-8.515	H
HETATM 956	N	0	-17.908	1.400	-3.145	N	HETATM 1044	H	0	-10.777	-3.354	-5.942	H
HETATM 957	C	0	-19.354	1.431	-3.450	C	HETATM 1045	H	0	-10.868	-8.540	-4.903	H
HETATM 958	C	0	-19.803	0.059	-3.948	C	HETATM 1046	H	0	-12.390	-9.591	-4.796	H
HETATM 959	O	0	-19.217	-0.511	-4.845	O	HETATM 1047	H	0	-9.925	-9.822	-3.238	H
HETATM 960	C	0	-19.637	2.534	-4.490	C	HETATM 1048	H	0	-11.411	-10.927	-3.300	H

HETATM 1049	H	0	-12.675	-8.859	-2.556	H	HETATM 1137	H	0	-9.988	-0.446	3.032	H
HETATM 1050	H	0	-7.853	-5.767	-3.714	H	HETATM 1138	H	0	-10.143	-1.569	4.362	H
HETATM 1051	H	0	-8.923	-4.309	-3.309	H	HETATM 1139	H	0	-10.665	-2.034	2.760	H
HETATM 1052	H	0	-7.460	-3.862	-1.451	H	HETATM 1140	H	0	-10.198	1.506	3.800	H
HETATM 1053	H	0	-5.353	-4.983	-1.169	H	HETATM 1141	H	0	-12.542	4.654	0.270	H
HETATM 1054	H	0	-6.697	-6.076	-0.943	H	HETATM 1142	H	0	-11.883	3.061	-0.409	H
HETATM 1055	H	0	-5.775	-6.120	-2.427	H	HETATM 1143	H	0	-7.022	6.734	1.958	H
HETATM 1056	H	0	-5.582	-3.024	-2.813	H	HETATM 1144	H	0	-8.417	5.983	2.919	H
HETATM 1057	H	0	-6.063	-4.074	-4.124	H	HETATM 1145	H	0	-8.600	6.434	0.000	H
HETATM 1058	H	0	-7.105	-2.763	-3.627	H	HETATM 1146	H	0	-6.017	0.706	1.872	H
HETATM 1059	H	0	-8.598	-6.815	-1.706	H	HETATM 1147	H	0	-7.752	1.291	2.158	H
HETATM 1060	H	0	-13.184	-2.550	0.351	H	HETATM 1148	H	0	-8.175	2.488	4.433	H
HETATM 1061	H	0	-12.503	-2.385	-1.250	H	HETATM 1149	H	0	-3.588	1.675	2.293	H
HETATM 1062	H	0	-13.446	-3.798	-0.843	H	HETATM 1150	H	0	-1.564	2.375	3.536	H
HETATM 1063	H	0	-10.786	-3.043	0.342	H	HETATM 1151	H	0	-3.922	3.711	6.845	H
HETATM 1064	H	0	-13.593	-8.815	1.896	H	HETATM 1152	H	0	-1.739	3.414	5.749	H
HETATM 1065	H	0	-12.754	-8.494	0.397	H	HETATM 1153	H	0	-5.556	2.923	0.949	H
HETATM 1066	H	0	-14.274	-7.700	0.735	H	HETATM 1154	H	0	-7.371	3.881	2.064	H
HETATM 1067	H	0	-13.252	-6.493	2.571	H	HETATM 1155	H	0	-10.465	1.459	-2.037	H
HETATM 1068	H	0	-7.256	-9.042	1.670	H	HETATM 1156	H	0	-9.303	0.156	-4.247	H
HETATM 1069	H	0	-7.967	-7.873	0.583	H	HETATM 1157	H	0	-10.492	-0.927	-3.565	H
HETATM 1070	H	0	-8.619	-9.492	0.673	H	HETATM 1158	H	0	-10.956	0.686	-4.049	H
HETATM 1071	H	0	-9.316	-9.109	2.939	H	HETATM 1159	H	0	-9.220	-0.660	-0.599	H
HETATM 1072	H	0	-7.817	-2.730	3.443	H	HETATM 1160	H	0	-10.887	-0.146	-0.503	H
HETATM 1073	H	0	-8.867	-3.531	2.143	H	HETATM 1161	H	0	-10.417	-1.377	-1.651	H
HETATM 1074	H	0	-5.936	-3.328	2.347	H	HETATM 1162	H	0	-7.731	0.199	-2.184	H
HETATM 1075	H	0	-6.924	-4.289	1.108	H	HETATM 1163	H	0	-2.385	4.384	-1.822	H
HETATM 1076	H	0	-4.640	-2.704	0.529	H	HETATM 1164	H	0	-3.758	5.318	-1.277	H
HETATM 1077	H	0	-4.785	-0.967	0.404	H	HETATM 1165	H	0	-3.775	3.576	-1.138	H
HETATM 1078	H	0	-5.207	-1.979	-0.956	H	HETATM 1166	H	0	-3.763	5.157	-3.682	H
HETATM 1079	H	0	-6.928	-5.062	3.735	H	HETATM 1167	H	0	-5.002	-0.203	-2.781	H
HETATM 1080	H	0	-12.437	-3.897	5.197	H	HETATM 1168	H	0	-3.603	-1.174	-3.172	H
HETATM 1081	H	0	-12.477	-5.742	5.366	H	HETATM 1169	H	0	-4.922	-1.045	-4.310	H
HETATM 1082	H	0	-12.783	-3.737	7.509	H	HETATM 1170	H	0	-2.633	0.615	-4.072	H
HETATM 1083	H	0	-13.008	-5.576	7.555	H	HETATM 1171	H	0	-6.741	2.944	-7.116	H
HETATM 1084	H	0	-14.643	-3.557	6.142	H	HETATM 1172	H	0	-7.559	1.300	-7.364	H
HETATM 1085	H	0	-14.880	-5.392	6.241	H	HETATM 1173	H	0	-6.339	2.872	-9.478	H
HETATM 1086	H	0	-14.930	-3.471	8.490	H	HETATM 1174	H	0	-8.115	2.989	-8.962	H
HETATM 1087	H	0	-15.403	-5.262	8.436	H	HETATM 1175	H	0	-6.675	0.584	-9.923	H
HETATM 1088	H	0	-17.286	-3.810	8.535	H	HETATM 1176	H	0	-8.477	0.822	-9.566	H
HETATM 1089	H	0	-17.215	-4.631	7.125	H	HETATM 1177	H	0	-6.848	2.070	-11.706	H
HETATM 1090	H	0	-10.502	-3.867	6.566	H	HETATM 1178	H	0	-8.662	2.243	-11.367	H
HETATM 1091	H	0	-6.553	-4.387	10.517	H	HETATM 1179	H	0	-7.348	0.363	-12.902	H
HETATM 1092	H	0	-8.341	-4.080	10.140	H	HETATM 1180	H	0	-8.946	0.516	-12.604	H
HETATM 1093	H	0	-6.547	-0.347	5.576	H	HETATM 1181	H	0	-5.510	0.341	-7.931	H
HETATM 1094	H	0	-6.814	-2.180	5.632	H	HETATM 1182	H	0	-3.520	5.712	-7.196	H
HETATM 1095	H	0	-4.610	-2.499	6.167	H	HETATM 1183	H	0	-2.727	6.175	-8.805	H
HETATM 1096	H	0	-3.515	-1.575	4.118	H	HETATM 1184	H	0	-5.529	6.757	-6.991	H
HETATM 1097	H	0	-4.839	-0.450	3.940	H	HETATM 1185	H	0	-4.392	5.169	-10.781	H
HETATM 1098	H	0	-5.121	-2.166	3.768	H	HETATM 1186	H	0	-7.711	7.399	-7.909	H
HETATM 1099	H	0	-2.899	-0.764	6.414	H	HETATM 1187	H	0	-6.656	5.706	-11.684	H
HETATM 1100	H	0	-4.115	-0.670	7.666	H	HETATM 1188	H	0	-8.305	6.823	-10.207	H
HETATM 1101	H	0	-4.138	0.466	6.339	H	HETATM 1189	H	0	-3.243	3.942	-9.553	H
HETATM 1102	H	0	-6.062	-0.786	8.110	H	HETATM 1190	H	0	1.248	1.865	-5.473	H
HETATM 1103	H	0	-11.672	-1.272	8.655	H	HETATM 1191	H	0	-0.581	1.800	-5.183	H
HETATM 1104	H	0	-11.556	-1.495	6.819	H	HETATM 1192	H	0	0.624	3.172	-3.610	H
HETATM 1105	H	0	-10.449	0.627	6.737	H	HETATM 1193	H	0	-0.514	4.114	-4.729	H
HETATM 1106	H	0	-10.793	4.079	11.212	H	HETATM 1194	H	0	0.668	3.483	-7.282	H
HETATM 1107	H	0	-11.770	2.802	10.291	H	HETATM 1195	H	0	0.632	-1.456	-6.629	H
HETATM 1108	H	0	-9.799	4.208	8.700	H	HETATM 1196	H	0	0.242	-2.826	-7.814	H
HETATM 1109	H	0	-5.146	2.070	8.846	H	HETATM 1197	H	0	-1.136	-2.728	-5.951	H
HETATM 1110	H	0	-5.957	0.700	9.794	H	HETATM 1198	H	0	0.671	-0.704	-9.046	H
HETATM 1111	H	0	-5.008	-0.077	11.850	H	HETATM 1199	H	0	-2.697	-0.545	-12.092	H
HETATM 1112	H	0	-3.116	3.026	9.631	H	HETATM 1200	H	0	-2.917	-2.379	-11.941	H
HETATM 1113	H	0	-2.975	-0.321	13.245	H	HETATM 1201	H	0	-4.319	-0.504	-10.198	H
HETATM 1114	H	0	-1.081	2.768	11.010	H	HETATM 1202	H	0	-6.072	-4.889	-7.205	H
HETATM 1115	H	0	-0.167	1.802	12.855	H	HETATM 1203	H	0	-5.872	-4.246	-8.931	H
HETATM 1116	H	0	-6.529	2.387	11.452	H	HETATM 1204	H	0	-5.771	-2.305	-5.793	H
HETATM 1117	H	0	-7.899	8.562	10.777	H	HETATM 1205	H	0	-8.018	-3.456	-9.225	H
HETATM 1118	H	0	-9.170	7.236	11.026	H	HETATM 1206	H	0	-7.433	-0.557	-5.284	H
HETATM 1119	H	0	-6.238	5.604	6.769	H	HETATM 1207	H	0	-9.728	-1.822	-8.675	H
HETATM 1120	H	0	-6.954	6.189	5.163	H	HETATM 1208	H	0	-9.399	-0.264	-6.767	H
HETATM 1121	H	0	-6.664	8.465	4.466	H	HETATM 1209	H	0	-4.152	-3.534	-6.569	H
HETATM 1122	H	0	-4.868	7.017	8.084	H	HETATM 1210	H	0	-0.080	-4.962	-9.919	H
HETATM 1123	H	0	-5.170	10.448	4.516	H	HETATM 1211	H	0	-1.566	-5.677	-10.764	H
HETATM 1124	H	0	-3.380	9.002	8.144	H	HETATM 1212	H	0	-1.962	-6.950	-8.772	H
HETATM 1125	H	0	-2.901	11.058	7.132	H	HETATM 1213	H	0	0.874	-8.875	-4.114	H
HETATM 1126	H	0	-8.461	7.569	6.567	H	HETATM 1214	H	0	-1.415	-9.630	-3.807	H
HETATM 1127	H	0	-12.793	6.498	5.812	H	HETATM 1215	H	0	-1.317	-7.885	-3.783	H
HETATM 1128	H	0	-13.221	5.030	4.765	H	HETATM 1216	H	0	-1.913	-8.708	-5.205	H
HETATM 1129	H	0	-11.272	6.442	3.699	H	HETATM 1217	H	0	0.152	-10.790	-5.255	H
HETATM 1130	H	0	-11.546	4.522	6.464	H	HETATM 1218	H	0	0.404	-6.695	-5.195	H
HETATM 1131	H	0	-12.944	1.121	4.116	H	HETATM 1219	H	0	4.550	-9.544	-9.368	H
HETATM 1132	H	0	-12.473	0.764	2.359	H	HETATM 1220	H	0	2.804	-9.140	-9.842	H
HETATM 1133	H	0	-12.043	-0.747	4.821	H	HETATM 1221	H	0	3.626	-10.943	-7.630	H
HETATM 1134	H	0	-13.007	-2.554	3.405	H	HETATM 1222	H	0	1.984	-10.727	-8.461	H
HETATM 1135	H	0	-14.092	-1.193	3.559	H	HETATM 1223	H	0	4.061	-8.570	-7.189	H
HETATM 1136	H	0	-13.169	-1.413	2.092	H	HETATM 1224	H	0	3.424	-2.578	-9.466	H

HETATM 1225	H	0	2.900	-3.308	-7.968	H	HETATM 1313	H	0	4.066	-0.418	0.195	H
HETATM 1226	H	0	2.106	-3.724	-9.467	H	HETATM 1314	H	0	4.972	-2.160	2.195	H
HETATM 1227	H	0	4.184	-4.795	-10.274	H	HETATM 1315	H	0	4.000	-0.949	2.996	H
HETATM 1228	H	0	9.679	-3.928	-8.653	H	HETATM 1316	H	0	3.326	-1.881	1.680	H
HETATM 1229	H	0	9.348	-6.331	-8.176	H	HETATM 1317	H	0	6.291	1.313	-0.220	H
HETATM 1230	H	0	8.413	-5.323	-7.098	H	HETATM 1318	H	0	10.298	3.599	-0.033	H
HETATM 1231	H	0	7.632	-6.134	-8.434	H	HETATM 1319	H	0	9.165	3.717	-1.495	H
HETATM 1232	H	0	9.641	-5.609	-10.351	H	HETATM 1320	H	0	10.083	1.466	-2.111	H
HETATM 1233	H	0	7.535	-3.079	-7.942	H	HETATM 1321	H	0	14.922	-1.305	-0.911	H
HETATM 1234	H	0	7.436	1.129	-9.214	H	HETATM 1322	H	0	13.384	-1.607	-1.900	H
HETATM 1235	H	0	8.251	1.907	-10.686	H	HETATM 1323	H	0	14.235	0.844	-2.292	H
HETATM 1236	H	0	9.110	-0.356	-11.152	H	HETATM 1324	H	0	12.870	-0.758	0.350	H
HETATM 1237	H	0	13.521	1.756	-11.826	H	HETATM 1325	H	0	13.266	4.754	0.442	H
HETATM 1238	H	0	13.503	-0.006	-11.253	H	HETATM 1326	H	0	14.333	4.623	-1.068	H
HETATM 1239	H	0	15.023	2.021	-9.790	H	HETATM 1327	H	0	15.553	5.721	1.283	H
HETATM 1240	H	0	15.711	1.236	-11.321	H	HETATM 1328	H	0	14.247	6.741	0.454	H
HETATM 1241	H	0	14.683	-0.097	-8.916	H	HETATM 1329	H	0	16.021	7.442	-0.632	H
HETATM 1242	H	0	15.529	-0.806	-10.404	H	HETATM 1330	H	0	15.689	5.865	-1.548	H
HETATM 1243	H	0	12.776	0.977	-9.074	H	HETATM 1331	H	0	17.537	5.873	0.674	H
HETATM 1244	H	0	13.662	4.659	-6.653	H	HETATM 1332	H	0	15.827	3.256	0.212	H
HETATM 1245	H	0	12.814	6.257	-7.056	H	HETATM 1333	H	0	12.062	4.032	5.360	H
HETATM 1246	H	0	12.194	5.347	-9.171	H	HETATM 1334	H	0	11.480	3.975	3.602	H
HETATM 1247	H	0	16.126	9.327	-10.831	H	HETATM 1335	H	0	11.849	6.104	2.283	H
HETATM 1248	H	0	14.024	9.845	-11.975	H	HETATM 1336	H	0	14.429	4.720	6.467	H
HETATM 1249	H	0	14.637	8.287	-12.474	H	HETATM 1337	H	0	16.131	6.271	7.400	H
HETATM 1250	H	0	13.316	8.382	-11.335	H	HETATM 1338	H	0	15.327	9.123	4.306	H
HETATM 1251	H	0	14.532	9.033	-8.672	H	HETATM 1339	H	0	16.574	8.434	6.311	H
HETATM 1252	H	0	15.745	6.839	-10.943	H	HETATM 1340	H	0	14.256	3.138	4.446	H
HETATM 1253	H	0	18.005	7.803	-4.927	H	HETATM 1341	H	0	8.912	-0.195	4.574	H
HETATM 1254	H	0	16.630	8.698	-5.789	H	HETATM 1342	H	0	9.582	0.269	2.909	H
HETATM 1255	H	0	18.374	7.777	-7.283	H	HETATM 1343	H	0	9.189	2.644	2.230	H
HETATM 1256	H	0	19.090	3.459	-6.955	H	HETATM 1344	H	0	9.128	0.937	7.009	H
HETATM 1257	H	0	17.918	3.000	-8.315	H	HETATM 1345	H	0	8.592	2.544	8.835	H
HETATM 1258	H	0	15.702	3.635	-3.120	H	HETATM 1346	H	0	8.162	5.757	6.035	H
HETATM 1259	H	0	14.268	2.461	-3.082	H	HETATM 1347	H	0	8.097	4.914	8.322	H
HETATM 1260	H	0	13.592	4.578	-3.444	H	HETATM 1348	H	0	11.128	0.259	5.503	H
HETATM 1261	H	0	16.114	1.549	-4.242	H	HETATM 1349	H	0	16.486	-5.160	4.022	H
HETATM 1262	H	0	13.101	-1.859	-5.439	H	HETATM 1350	H	0	15.792	-6.711	3.281	H
HETATM 1263	H	0	12.235	-2.933	-7.469	H	HETATM 1351	H	0	15.924	-3.994	2.052	H
HETATM 1264	H	0	10.988	-2.035	-6.636	H	HETATM 1352	H	0	14.400	-4.845	-2.163	H
HETATM 1265	H	0	11.729	-1.373	-8.074	H	HETATM 1353	H	0	15.458	-5.694	-3.427	H
HETATM 1266	H	0	14.478	-0.265	-7.116	H	HETATM 1354	H	0	15.677	-6.737	-1.314	H
HETATM 1267	H	0	12.351	0.729	-6.744	H	HETATM 1355	H	0	20.430	-5.780	-0.230	H
HETATM 1268	H	0	6.915	1.135	-5.074	H	HETATM 1356	H	0	19.941	-7.021	-1.516	H
HETATM 1269	H	0	7.998	1.376	-6.559	H	HETATM 1357	H	0	20.686	-3.297	-5.961	H
HETATM 1270	H	0	8.967	0.380	-3.936	H	HETATM 1358	H	0	20.403	-4.980	-5.238	H
HETATM 1271	H	0	7.987	-3.561	-2.369	H	HETATM 1359	H	0	18.400	-2.828	-5.326	H
HETATM 1272	H	0	7.560	-5.018	-3.431	H	HETATM 1360	H	0	18.221	-4.662	-5.127	H
HETATM 1273	H	0	9.142	-5.950	-4.893	H	HETATM 1361	H	0	19.225	-3.339	-7.550	H
HETATM 1274	H	0	10.047	-2.356	-2.752	H	HETATM 1362	H	0	18.478	-5.014	-7.288	H
HETATM 1275	H	0	11.512	-6.105	-5.612	H	HETATM 1363	H	0	21.612	-3.447	-3.716	H
HETATM 1276	H	0	12.408	-2.523	-3.447	H	HETATM 1364	H	0	17.989	-0.081	-0.903	H
HETATM 1277	H	0	13.918	-3.739	-4.509	H	HETATM 1365	H	0	18.697	2.244	-2.294	H
HETATM 1278	H	0	7.229	-3.402	-5.283	H	HETATM 1366	H	0	17.540	2.048	-0.999	H
HETATM 1279	H	0	3.739	-4.675	-3.170	H	HETATM 1367	H	0	17.030	1.873	-2.661	H
HETATM 1280	H	0	3.426	-5.354	-4.865	H	HETATM 1368	H	0	17.824	-1.071	-3.362	H
HETATM 1281	H	0	-1.989	-3.301	-3.145	H	HETATM 1369	H	0	19.794	0.458	-3.273	H
HETATM 1282	H	0	-1.176	-5.180	-4.992	H	HETATM 1370	H	0	24.710	2.133	-1.197	H
HETATM 1283	H	0	-1.671	-6.027	-3.545	H	HETATM 1371	H	0	23.375	3.138	-1.998	H
HETATM 1284	H	0	-2.760	-4.895	-4.311	H	HETATM 1372	H	0	24.239	0.307	-2.627	H
HETATM 1285	H	0	-0.384	-3.384	-1.372	H	HETATM 1373	H	0	24.130	1.765	-3.767	H
HETATM 1286	H	0	-0.366	-5.204	-1.719	H	HETATM 1374	H	0	21.855	1.780	-3.664	H
HETATM 1287	H	0	-1.914	-4.625	0.114	H	HETATM 1375	H	0	22.140	-0.039	-3.448	H
HETATM 1288	H	0	-2.756	-3.539	-0.964	H	HETATM 1376	H	0	23.094	0.749	-0.149	H
HETATM 1289	H	0	-2.739	-5.255	-1.291	H	HETATM 1377	H	0	23.041	3.189	3.326	H
HETATM 1290	H	0	-0.102	-3.355	-5.022	H	HETATM 1378	H	0	22.551	4.378	1.991	H
HETATM 1291	H	0	0.920	0.996	-0.355	H	HETATM 1379	H	0	19.240	0.127	1.944	H
HETATM 1292	H	0	1.116	-0.829	-0.096	H	HETATM 1380	H	0	18.522	1.415	0.821	H
HETATM 1293	H	0	-1.227	-0.994	-0.875	H	HETATM 1381	H	0	16.936	0.866	2.818	H
HETATM 1294	H	0	-0.191	-0.364	1.693	H	HETATM 1382	H	0	18.411	2.939	2.616	H
HETATM 1295	H	0	-1.731	0.447	1.542	H	HETATM 1383	H	0	16.143	1.556	7.727	H
HETATM 1296	H	0	-1.628	-1.283	1.316	H	HETATM 1384	H	0	15.467	2.555	6.320	H
HETATM 1297	H	0	-0.964	1.770	-1.372	H	HETATM 1385	H	0	16.641	3.970	7.741	H
HETATM 1298	H	0	-2.162	1.580	-0.114	H	HETATM 1386	H	0	17.721	3.562	6.291	H
HETATM 1299	H	0	-2.358	0.751	-1.640	H	HETATM 1387	H	0	19.030	3.617	8.258	H
HETATM 1300	H	0	0.419	0.412	-2.699	H	HETATM 1388	H	0	18.698	1.856	7.786	H
HETATM 1301	H	0	5.056	1.936	-5.078	H	HETATM 1389	H	0	17.560	1.597	9.723	H
HETATM 1302	H	0	3.327	2.031	-4.416	H	HETATM 1390	H	0	17.756	0.641	6.287	H
HETATM 1303	H	0	3.346	1.622	-6.763	H	HETATM 1391	H	0	15.982	-3.217	7.185	H
HETATM 1304	H	0	2.860	0.110	-5.808	H	HETATM 1392	H	0	15.905	-3.137	5.335	H
HETATM 1305	H	0	4.956	-1.890	-7.466	H	HETATM 1393	H	0	13.993	-1.806	5.493	H
HETATM 1306	H	0	4.308	-1.734	-5.868	H	HETATM 1394	H	0	10.735	1.026	9.260	H
HETATM 1307	H	0	5.027	-0.392	-4.286	H	HETATM 1395	H	0	11.821	1.271	7.778	H
HETATM 1308	H	0	6.189	-1.653	0.135	H	HETATM 1396	H	0	11.817	2.437	10.373	H
HETATM 1309	H	0	7.945	0.109	1.428	H	HETATM 1397	H	0	14.226	2.612	10.627	H
HETATM 1310	H	0	6.708	-0.346	2.574	H	HETATM 1398	H	0	13.626	0.987	10.857	H
HETATM 1311	H	0	7.644	-1.579	1.765	H	HETATM 1399	H	0	14.427	1.420	9.366	H
HETATM 1312	H	0	4.781	0.570	1.591	H	HETATM 1400	H	0	13.068	4.166	9.212	H

HETATM 1401	H	0	13.111	3.149	7.791	H	HETATM 1489	H	0	-1.583	-6.123	5.843	H
HETATM 1402	H	0	11.582	3.736	8.400	H	HETATM 1490	H	0	-2.109	-3.587	7.026	H
HETATM 1403	H	0	12.808	-0.550	9.745	H	HETATM 1491	H	0	-2.663	-5.157	7.557	H
HETATM 1404	H	0	12.693	-7.043	10.450	H	HETATM 1492	H	0	-3.620	-4.228	6.428	H
HETATM 1405	H	0	11.020	-6.261	10.602	H	HETATM 1493	H	0	-2.356	-4.631	3.558	H
HETATM 1406	H	0	11.989	-3.387	12.064	H	HETATM 1494	H	0	-3.740	-4.760	4.616	H
HETATM 1407	H	0	10.974	-4.773	12.281	H	HETATM 1495	H	0	-2.928	-6.204	4.060	H
HETATM 1408	H	0	13.087	-5.650	8.508	H	HETATM 1496	H	0	-0.963	-3.387	4.715	H
HETATM 1409	H	0	9.365	-8.202	4.515	H	HETATM 1497	H	0	2.891	-5.501	9.645	H
HETATM 1410	H	0	9.267	-8.635	7.263	H	HETATM 1498	H	0	2.850	-6.251	7.950	H
HETATM 1411	H	0	8.071	-7.423	6.873	H	HETATM 1499	H	0	0.884	-4.283	8.976	H
HETATM 1412	H	0	8.054	-8.964	6.050	H	HETATM 1500	H	0	0.095	0.798	4.235	H
HETATM 1413	H	0	9.369	-5.620	5.913	H	HETATM 1501	H	0	1.050	-0.450	3.471	H
HETATM 1414	H	0	10.094	-5.947	4.239	H	HETATM 1502	H	0	-0.024	-0.855	4.788	H
HETATM 1415	H	0	7.919	-4.838	4.106	H	HETATM 1503	H	0	2.452	0.849	4.974	H
HETATM 1416	H	0	7.211	-6.147	5.023	H	HETATM 1504	H	0	-0.062	-0.151	10.915	H
HETATM 1417	H	0	7.895	-6.455	3.444	H	HETATM 1505	H	0	0.780	-1.383	9.816	H
HETATM 1418	H	0	11.238	-8.802	6.236	H	HETATM 1506	H	0	-2.026	-0.455	9.849	H
HETATM 1419	H	0	13.874	-10.433	2.050	H	HETATM 1507	H	0	-1.212	-1.492	8.546	H
HETATM 1420	H	0	12.343	-10.359	1.008	H	HETATM 1508	H	0	-1.694	-2.188	11.403	H
HETATM 1421	H	0	12.804	-11.795	3.321	H	HETATM 1509	H	0	-0.962	-3.230	10.057	H
HETATM 1422	H	0	11.194	-11.397	2.495	H	HETATM 1510	H	0	-3.707	-2.157	10.246	H
HETATM 1423	H	0	12.306	-10.525	4.975	H	HETATM 1511	H	0	-2.966	-3.282	8.972	H
HETATM 1424	H	0	10.639	-10.245	4.216	H	HETATM 1512	H	0	-2.767	-4.418	11.440	H
HETATM 1425	H	0	13.499	-8.179	2.288	H	HETATM 1513	H	0	-4.321	-3.935	11.298	H
HETATM 1426	H	0	11.740	-10.666	-2.818	H	HETATM 1514	H	0	-0.308	1.215	8.873	H
HETATM 1427	H	0	10.263	-11.784	-2.791	H	HETATM 1515	H	0	6.132	1.365	10.197	H
HETATM 1428	H	0	10.909	-11.217	-0.351	H	HETATM 1516	H	0	5.311	0.286	8.933	H
HETATM 1429	H	0	9.645	-9.455	-2.977	H	HETATM 1517	H	0	5.469	0.019	11.830	H
HETATM 1430	H	0	8.781	-10.000	2.454	H	HETATM 1518	H	0	4.500	-1.010	10.631	H
HETATM 1431	H	0	7.123	-9.530	2.740	H	HETATM 1519	H	0	7.429	-0.799	11.072	H
HETATM 1432	H	0	7.577	-11.216	2.808	H	HETATM 1520	H	0	6.626	-1.506	9.558	H
HETATM 1433	H	0	7.194	-11.431	0.609	H	HETATM 1521	H	0	7.302	-3.199	11.192	H
HETATM 1434	H	0	7.002	-6.059	-1.165	H	HETATM 1522	H	0	5.465	-3.028	11.019	H
HETATM 1435	H	0	5.377	-5.323	-0.661	H	HETATM 1523	H	0	6.372	-1.363	12.967	H
HETATM 1436	H	0	7.501	-6.288	1.212	H	HETATM 1524	H	0	7.029	-2.821	13.297	H
HETATM 1437	H	0	7.922	-3.887	1.545	H	HETATM 1525	H	0	3.847	1.826	11.018	H
HETATM 1438	H	0	8.245	-4.332	-0.114	H	HETATM 1526	H	0	3.346	3.095	5.403	H
HETATM 1439	H	0	6.762	-3.504	0.296	H	HETATM 1527	H	0	4.466	5.706	5.276	H
HETATM 1440	H	0	6.086	-5.147	2.853	H	HETATM 1528	H	0	5.189	4.764	3.994	H
HETATM 1441	H	0	4.951	-4.715	1.596	H	HETATM 1529	H	0	3.451	4.922	4.089	H
HETATM 1442	H	0	5.176	-6.392	2.032	H	HETATM 1530	H	0	6.261	3.269	4.925	H
HETATM 1443	H	0	4.788	-7.412	0.300	H	HETATM 1531	H	0	5.493	1.919	5.936	H
HETATM 1444	H	0	6.472	-10.336	-4.203	H	HETATM 1532	H	0	6.046	1.201	3.698	H
HETATM 1445	H	0	5.451	-9.706	-5.615	H	HETATM 1533	H	0	5.051	2.484	3.054	H
HETATM 1446	H	0	7.422	-8.227	-3.950	H	HETATM 1534	H	0	4.326	1.211	4.006	H
HETATM 1447	H	0	8.568	-8.059	-6.174	H	HETATM 1535	H	0	5.394	4.329	7.229	H
HETATM 1448	H	0	8.361	-9.731	-5.709	H	HETATM 1536	H	0	-0.206	4.514	6.407	H
HETATM 1449	H	0	7.288	-9.013	-6.886	H	HETATM 1537	H	0	-0.097	4.064	9.175	H
HETATM 1450	H	0	6.987	-6.321	-5.359	H	HETATM 1538	H	0	-1.749	4.475	8.781	H
HETATM 1451	H	0	5.574	-6.783	-4.441	H	HETATM 1539	H	0	-0.958	3.152	7.959	H
HETATM 1452	H	0	5.683	-7.185	-6.138	H	HETATM 1540	H	0	-0.849	7.179	7.049	H
HETATM 1453	H	0	4.182	-8.408	-4.033	H	HETATM 1541	H	0	-2.155	6.176	7.633	H
HETATM 1454	H	0	4.186	-12.792	-0.597	H	HETATM 1542	H	0	-1.679	6.101	5.953	H
HETATM 1455	H	0	2.663	-11.997	-0.043	H	HETATM 1543	H	0	1.247	6.537	7.014	H
HETATM 1456	H	0	2.670	-14.240	0.315	H	HETATM 1544	H	0	2.181	5.295	13.294	H
HETATM 1457	H	0	3.262	-12.956	-2.910	H	HETATM 1545	H	0	2.919	4.267	11.941	H
HETATM 1458	H	0	-0.875	-14.411	-4.752	H	HETATM 1546	H	0	0.999	3.435	12.981	H
HETATM 1459	H	0	-2.430	-14.250	-3.881	H	HETATM 1547	H	0	1.136	6.634	11.571	H
HETATM 1460	H	0	-1.691	-15.528	-2.292	H	HETATM 1548	H	0	7.324	7.640	10.211	H
HETATM 1461	H	0	-1.074	-12.154	-3.810	H	HETATM 1549	H	0	6.226	6.222	9.745	H
HETATM 1462	H	0	0.376	-13.893	1.585	H	HETATM 1550	H	0	5.562	7.580	11.751	H
HETATM 1463	H	0	-1.133	-14.861	1.606	H	HETATM 1551	H	0	4.947	11.762	10.823	H
HETATM 1464	H	0	-2.471	-12.938	0.842	H	HETATM 1552	H	0	3.325	11.552	11.695	H
HETATM 1465	H	0	-2.161	-7.093	1.220	H	HETATM 1553	H	0	4.246	11.672	6.048	H
HETATM 1466	H	0	-2.400	-9.172	-0.708	H	HETATM 1554	H	0	3.200	13.077	5.443	H
HETATM 1467	H	0	-2.845	-7.493	-0.891	H	HETATM 1555	H	0	2.400	13.257	7.754	H
HETATM 1468	H	0	-4.019	-8.649	-0.311	H	HETATM 1556	H	0	-0.370	9.198	7.798	H
HETATM 1469	H	0	-3.300	-7.985	3.129	H	HETATM 1557	H	0	-0.972	10.768	7.019	H
HETATM 1470	H	0	-4.226	-9.079	1.953	H	HETATM 1558	H	0	-3.087	9.218	3.322	H
HETATM 1471	H	0	-5.535	-7.205	2.702	H	HETATM 1559	H	0	-2.319	8.028	2.127	H
HETATM 1472	H	0	-4.302	-6.122	2.102	H	HETATM 1560	H	0	-3.369	7.637	4.841	H
HETATM 1473	H	0	-5.175	-7.153	0.993	H	HETATM 1561	H	0	-2.244	6.473	3.939	H
HETATM 1474	H	0	-0.571	-8.914	0.882	H	HETATM 1562	H	0	-2.620	5.718	1.778	H
HETATM 1475	H	0	0.623	-11.370	5.605	H	HETATM 1563	H	0	-3.871	4.499	1.837	H
HETATM 1476	H	0	1.186	-10.146	7.613	H	HETATM 1564	H	0	-4.068	5.904	0.817	H
HETATM 1477	H	0	0.090	-11.469	8.108	H	HETATM 1565	H	0	-0.467	7.918	3.754	H
HETATM 1478	H	0	-0.554	-9.786	7.983	H	HETATM 1566	H	0	1.588	12.823	3.623	H
HETATM 1479	H	0	-1.206	-12.420	6.273	H	HETATM 1567	H	0	1.874	13.523	1.931	H
HETATM 1480	H	0	-1.173	-8.921	5.689	H	HETATM 1568	H	0	0.423	11.762	1.114	H
HETATM 1481	H	0	5.268	-8.303	4.075	H	HETATM 1569	H	0	4.743	7.306	2.913	H
HETATM 1482	H	0	4.532	-9.851	4.411	H	HETATM 1570	H	0	4.130	8.424	4.107	H
HETATM 1483	H	0	4.083	-8.965	2.974	H	HETATM 1571	H	0	3.031	7.365	3.256	H
HETATM 1484	H	0	3.529	-8.130	5.821	H	HETATM 1572	H	0	4.630	9.607	2.053	H
HETATM 1485	H	0	1.204	-4.167	1.110	H	HETATM 1573	H	0	0.166	7.069	-0.454	H
HETATM 1486	H	0	0.745	-5.949	1.331	H	HETATM 1574	H	0	0.740	6.339	-2.058	H
HETATM 1487	H	0	3.283	-5.779	0.809	H	HETATM 1575	H	0	2.344	4.225	-1.885	H
HETATM 1488	H	0	3.090	-4.719	2.605	H	HETATM 1576	H	0	0.102	6.705	2.003	H

HETATM 1577	H	0	0.014	5.561	4.228	H	HETATM 1665	H	0	-9.976	3.639	-9.802	H
HETATM 1578	H	0	2.048	2.148	2.648	H	HETATM 1666	H	0	-13.908	2.566	-5.418	H
HETATM 1579	H	0	0.982	3.324	4.526	H	HETATM 1667	H	0	-16.020	-0.122	0.052	H
HETATM 1580	H	0	2.950	7.105	-1.445	H	HETATM 1668	H	0	-13.850	0.640	0.910	H
HETATM 1581	H	0	4.629	10.790	-3.895	H	HETATM 1669	H	0	-13.539	1.448	-0.608	H
HETATM 1582	H	0	5.145	9.730	-6.016	H	HETATM 1670	H	0	-13.683	-0.293	-0.558	H
HETATM 1583	H	0	4.485	8.601	-4.857	H	HETATM 1671	H	0	-15.676	2.788	0.071	H
HETATM 1584	H	0	3.482	9.212	-6.150	H	HETATM 1672	H	0	-17.288	1.874	0.060	H
HETATM 1585	H	0	4.508	12.100	-5.991	H	HETATM 1673	H	0	-15.702	0.929	2.175	H
HETATM 1586	H	0	3.392	12.701	-4.788	H	HETATM 1674	H	0	-15.687	2.673	2.283	H
HETATM 1587	H	0	2.806	11.725	-6.114	H	HETATM 1675	H	0	-17.207	1.811	2.273	H
HETATM 1588	H	0	2.419	11.088	-3.125	H	HETATM 1676	H	0	-15.433	-0.154	-2.323	H
HETATM 1589	H	0	0.661	6.854	-6.419	H	HETATM 1677	H	0	-19.142	3.408	-4.120	H
HETATM 1590	H	0	-1.083	6.853	-6.317	H	HETATM 1678	H	0	-19.352	2.117	-5.433	H
HETATM 1591	H	0	-0.290	7.545	-7.712	H	HETATM 1679	H	0	-21.571	2.869	-3.679	H
HETATM 1592	H	0	-0.172	9.461	-6.754	H	HETATM 1680	H	0	-21.518	2.358	-5.459	H
HETATM 1593	H	0	-1.638	8.625	-1.112	H	HETATM 1681	H	0	-20.585	4.534	-5.914	H
HETATM 1594	H	0	-2.692	7.241	-1.752	H	HETATM 1682	H	0	-22.286	4.617	-5.182	H
HETATM 1595	H	0	-5.213	7.291	-1.138	H	HETATM 1683	H	0	-20.853	5.030	-3.079	H
HETATM 1596	H	0	-1.813	10.895	0.054	H	HETATM 1684	H	0	-19.912	1.658	-2.566	H
HETATM 1597	H	0	-2.408	12.558	1.788	H	HETATM 1685	H	0	-22.390	-1.771	-3.347	H
HETATM 1598	H	0	-6.328	10.902	2.204	H	HETATM 1686	H	0	-21.222	-1.808	-4.785	H
HETATM 1599	H	0	-4.682	12.645	2.733	H	HETATM 1687	H	0	-20.052	-8.583	-0.509	H
HETATM 1600	H	0	-3.431	8.589	-3.488	H	HETATM 1688	H	0	-21.721	-7.819	-0.247	H
HETATM 1601	H	0	-0.008	12.808	-1.241	H	HETATM 1689	H	0	-21.227	-8.302	2.145	H
HETATM 1602	H	0	0.267	13.210	-3.029	H	HETATM 1690	H	0	-20.087	-9.569	1.417	H
HETATM 1603	H	0	-1.079	14.866	-0.989	H	HETATM 1691	H	0	-21.799	-10.854	1.631	H
HETATM 1604	H	0	-0.640	15.269	-2.744	H	HETATM 1692	H	0	-22.982	-9.428	1.621	H
HETATM 1605	H	0	1.071	15.055	-0.333	H	HETATM 1693	H	0	-23.470	-10.037	-0.449	H
HETATM 1606	H	0	0.891	16.430	-1.562	H	HETATM 1694	H	0	-20.796	-6.182	1.025	H
HETATM 1607	H	0	2.635	14.143	-1.654	H	HETATM 1695	H	0	-16.214	-4.604	3.927	H
HETATM 1608	H	0	-2.361	12.859	-1.687	H	HETATM 1696	H	0	-18.030	-4.245	3.822	H
HETATM 1609	H	0	-0.645	12.206	-7.090	H	HETATM 1697	H	0	-17.630	-3.798	1.454	H
HETATM 1610	H	0	-1.242	13.617	-8.133	H	HETATM 1698	H	0	-17.136	-2.215	3.742	H
HETATM 1611	H	0	-2.172	14.526	-5.999	H	HETATM 1699	H	0	-15.992	-1.748	2.506	H
HETATM 1612	H	0	-4.186	9.297	-7.417	H	HETATM 1700	H	0	-17.706	-1.702	2.172	H
HETATM 1613	H	0	-5.398	9.865	-8.700	H	HETATM 1701	H	0	-15.072	-4.798	2.080	H
HETATM 1614	H	0	-2.638	10.841	-8.300	H	HETATM 1702	H	0	-14.898	-3.124	1.612	H
HETATM 1615	H	0	-3.834	11.167	-9.678	H	HETATM 1703	H	0	-15.680	-4.255	0.535	H
HETATM 1616	H	0	-1.959	9.736	-10.251	H	HETATM 1704	H	0	-16.643	-6.469	2.426	H
HETATM 1617	H	0	-2.717	8.531	-9.064	H	HETATM 1705	H	0	-14.271	-4.307	-3.123	H
HETATM 1618	H	0	-4.677	9.367	-10.788	H	HETATM 1706	H	0	-16.113	-5.896	-3.069	H
HETATM 1619	H	0	-5.374	12.033	-7.733	H	HETATM 1707	H	0	-15.683	-6.278	-4.831	H
HETATM 1620	H	0	-4.654	12.896	-0.769	H	HETATM 1708	H	0	-11.842	-12.171	10.232	H
HETATM 1621	H	0	-5.129	14.261	-1.929	H	HETATM 1709	H	0	-13.279	-13.973	9.597	H
HETATM 1622	H	0	-5.680	14.096	0.969	H	HETATM 1710	H	0	-13.027	-12.934	8.322	H
HETATM 1623	H	0	-5.934	15.499	-0.215	H	HETATM 1711	H	0	-11.636	-14.314	11.239	H
HETATM 1624	H	0	-3.378	14.242	0.620	H	HETATM 1712	H	0	-10.167	-13.534	11.159	H
HETATM 1625	H	0	-3.655	15.686	-0.509	H	HETATM 1713	H	0	-6.168	-7.984	8.509	H
HETATM 1626	H	0	-4.086	15.497	2.418	H	HETATM 1714	H	0	-4.389	-7.112	7.042	H
HETATM 1627	H	0	-4.413	16.936	1.297	H	HETATM 1715	H	0	-5.735	-6.857	5.794	H
HETATM 1628	H	0	-2.373	17.139	2.496	H	HETATM 1716	H	0	-3.640	-9.351	7.685	H
HETATM 1629	H	0	-2.134	16.992	0.888	H	HETATM 1717	H	0	-6.672	-9.565	4.754	H
HETATM 1630	H	0	-7.036	12.487	-0.474	H	HETATM 1718	H	0	-3.945	-11.802	7.100	H
HETATM 1631	H	0	-10.227	15.387	-0.312	H	HETATM 1719	H	0	-0.296	4.746	13.968	H
HETATM 1632	H	0	-9.281	15.968	-1.795	H	HETATM 1720	H	0	-1.927	4.242	15.593	H
HETATM 1633	H	0	-11.755	12.047	-5.681	H	HETATM 1721	H	0	-2.479	5.779	15.593	H
HETATM 1634	H	0	-9.776	13.878	-4.956	H	HETATM 1722	H	0	0.322	6.871	15.608	H
HETATM 1635	H	0	-8.994	12.364	-5.341	H	HETATM 1723	H	0	0.944	5.361	15.628	H
HETATM 1636	H	0	-10.052	13.122	-6.507	H	HETATM 1724	H	0	-8.197	4.077	-5.043	H
HETATM 1637	H	0	-10.933	10.821	-3.482	H	HETATM 1725	H	0	-7.791	5.970	-2.773	H
HETATM 1638	H	0	-12.203	13.889	-4.169	H	HETATM 1726	H	0	-9.406	5.588	-3.597	H
HETATM 1639	H	0	-16.458	12.043	-4.008	H	HETATM 1727	H	0	12.111	-3.765	4.076	H
HETATM 1640	H	0	-15.857	10.656	-5.080	H	HETATM 1728	H	0	11.433	-4.946	2.134	H
HETATM 1641	H	0	-15.090	11.239	-2.271	H	HETATM 1729	H	0	10.194	-3.677	2.672	H
HETATM 1642	H	0	-11.213	6.908	-1.050	H	HETATM 1730	H	0	8.933	-2.804	9.165	H
HETATM 1643	H	0	-9.698	8.845	-0.946	H	HETATM 1731	H	0	9.190	-3.062	6.200	H
HETATM 1644	H	0	-10.924	9.840	-1.694	H	HETATM 1732	H	0	7.892	-3.925	7.201	H
HETATM 1645	H	0	-10.204	8.522	-2.587	H	HETATM 1733	H	0	10.260	-6.016	0.364	H
HETATM 1646	H	0	-11.208	8.292	0.957	H	HETATM 1734	H	0	12.403	-6.207	-1.686	H
HETATM 1647	H	0	-12.487	9.273	0.282	H	HETATM 1735	H	0	10.883	-5.151	-1.770	H
HETATM 1648	H	0	-12.782	7.593	0.664	H	HETATM 1736	H	0	4.902	-2.306	7.520	H
HETATM 1649	H	0	-12.474	7.665	-3.050	H	HETATM 1737	H	0	5.677	-3.816	5.854	H
HETATM 1650	H	0	-16.707	7.664	0.428	H	HETATM 1738	H	0	4.634	-2.904	4.622	H
HETATM 1651	H	0	-17.745	7.250	-1.050	H	HETATM 1739	H	0	-7.847	10.058	-4.658	H
HETATM 1652	H	0	-17.595	5.879	1.527	H	HETATM 1740	H	0	-5.612	9.269	-2.798	H
HETATM 1653	H	0	-18.673	5.533	0.060	H	HETATM 1741	H	0	-7.369	8.694	-2.672	H
HETATM 1654	H	0	-15.635	5.415	-0.117	H	HETATM 1742	H	0	-18.958	-4.769	-2.790	H
HETATM 1655	H	0	-16.063	7.316	-5.351	H	HETATM 1743	H	0	-17.488	-2.984	-0.897	H
HETATM 1656	H	0	-15.714	5.943	-6.374	H	HETATM 1744	H	0	-16.956	-4.638	-1.540	H
HETATM 1657	H	0	-17.351	6.540	-6.242	H	HETATM 1745	H	0	-3.799	-13.796	6.161	H
HETATM 1658	H	0	-17.732	5.213	-4.473	H	HETATM 1746	H	0	-7.083	-12.700	7.482	H
HETATM 1659	H	0	-12.534	3.641	-2.988	H	HETATM 1747	H	0	-8.639	-10.829	7.556	H
HETATM 1660	H	0	-11.930	2.172	-3.943	H	HETATM 1748	H	0	-9.618	-11.721	6.354	H
HETATM 1661	H	0	-11.794	5.900	-3.883	H	HETATM 1749	H	0	-10.636	-10.517	8.998	H
HETATM 1662	H	0	-11.736	1.537	-6.490	H	HETATM 1750	H	0	-11.696	-11.212	7.707	H
HETATM 1663	H	0	-10.836	1.536	-8.793	H	HETATM 1751	C	0	-3.539	6.174	10.915	C
HETATM 1664	H	0	-9.944	5.735	-8.529	H	HETATM 1752	C	0	-4.945	5.970	11.532	C

HETATM 1753	C	0	-9.970	-9.589	6.346	C	HETATM 1841	H	0	19.785	-2.077	-1.765	H
HETATM 1754	H	0	-9.212	-9.455	5.546	H	HETATM 1842	H	0	18.263	-5.172	-0.120	H
HETATM 1755	H	0	-10.959	-9.694	5.848	H	HETATM 1843	H	0	23.136	1.571	1.735	H
HETATM 1756	C	0	-2.338	5.739	11.775	C	HETATM 1844	H	0	14.430	-2.813	-3.497	H
HETATM 1757	H	0	-4.850	6.213	12.570	H	HETATM 1845	H	0	15.352	8.266	-3.771	H
HETATM 1758	H	0	-3.425	7.215	10.691	H	HETATM 1846	H	0	5.718	-0.006	-9.535	H
HETATM 1759	H	0	-3.500	5.630	9.995	H	HETATM 1847	H	0	4.990	-0.322	-10.962	H
HETATM 1760	H	0	-2.559	4.811	12.259	H	HETATM 1848	H	0	8.706	-1.122	-8.340	H
HETATM 1761	H	0	-1.473	5.626	11.156	H	HETATM 1849	H	0	6.216	-4.094	-10.393	H
HETATM 1762	H	0	-2.965	6.928	13.427	H	HETATM 1850	H	0	9.974	5.634	-6.843	H
HETATM 1763	H	0	-1.912	7.752	12.323	H	HETATM 1851	H	0	10.740	5.106	-8.185	H
HETATM 1764	H	0	-5.435	4.050	12.321	H	HETATM 1852	H	0	6.764	3.895	-4.843	H
HETATM 1765	H	0	3.847	10.772	8.316	H	HETATM 1853	H	0	13.270	2.448	-0.699	H
HETATM 1766	H	0	1.456	10.390	8.353	H	HETATM 1854	H	0	13.328	8.199	2.532	H
HETATM 1767	H	0	8.520	4.838	3.387	H	HETATM 1855	H	0	17.085	5.732	-2.665	H
HETATM 1768	H	0	-0.243	7.306	13.774	H	HETATM 1856	H	0	18.669	6.025	-2.936	H
HETATM 1769	H	0	2.638	-5.835	-8.140	H	HETATM 1857	H	0	19.452	4.699	0.269	H
HETATM 1770	H	0	1.656	8.176	-5.026	H	HETATM 1858	H	0	20.215	5.062	-1.236	H
HETATM 1771	H	0	-9.492	-12.558	9.181	H	HETATM 1859	H	0	12.817	2.676	1.954	H
HETATM 1772	C	0	-9.981	-8.329	7.238	C	HETATM 1860	H	0	16.189	3.214	11.816	H
HETATM 1773	H	0	-10.739	-8.454	7.984	H	HETATM 1861	H	0	17.714	2.684	12.300	H
HETATM 1774	H	0	-7.949	-7.132	6.334	H	HETATM 1862	H	0	17.262	5.334	10.478	H
HETATM 1775	H	0	-10.444	-7.243	5.466	H	HETATM 1863	H	0	18.236	4.846	9.261	H
HETATM 1776	H	0	-8.172	-5.540	8.422	H	HETATM 1864	H	0	16.852	2.502	4.185	H
HETATM 1777	H	0	-20.330	-11.032	0.161	H	HETATM 1865	H	0	20.904	1.552	2.202	H
HETATM 1778	H	0	-19.896	-10.626	-1.360	H	HETATM 1866	H	0	17.902	-7.793	3.336	H
HETATM 1779	H	0	-22.963	-11.851	-2.221	H	HETATM 1867	H	0	18.926	-7.417	2.121	H
HETATM 1780	H	0	-21.519	-11.478	-2.886	H	HETATM 1868	H	0	13.664	-5.350	3.286	H
HETATM 1781	H	0	-19.500	-5.826	2.722	H	HETATM 1869	H	0	16.399	-4.179	-0.043	H
HETATM 1782	H	0	-19.609	-6.495	-1.634	H	HETATM 1870	H	0	11.963	0.433	-2.031	H
HETATM 1783	H	0	-19.261	-1.950	-2.280	H	HETATM 1871	H	0	12.017	1.056	2.851	H
HETATM 1784	H	0	-21.205	-0.043	-2.500	H	HETATM 1872	H	0	15.884	-0.512	7.373	H
HETATM 1785	H	0	-19.471	8.147	-3.538	H	HETATM 1873	H	0	12.720	-4.882	6.688	H
HETATM 1786	H	0	-20.486	7.336	-2.549	H	HETATM 1874	H	0	13.001	-4.503	5.124	H
HETATM 1787	H	0	-20.585	7.731	-5.651	H	HETATM 1875	H	0	12.855	-0.168	6.912	H
HETATM 1788	H	0	-19.025	7.253	-5.586	H	HETATM 1876	H	0	10.469	5.849	-1.734	H
HETATM 1789	H	0	-17.290	1.996	-3.657	H	HETATM 1877	H	0	11.672	5.627	-2.960	H
HETATM 1790	H	0	-14.349	4.795	-3.762	H	HETATM 1878	H	0	8.238	2.003	0.099	H
HETATM 1791	H	0	-15.522	2.784	-2.385	H	HETATM 1879	H	0	10.852	-1.831	7.203	H
HETATM 1792	H	0	-16.021	7.018	-3.232	H	HETATM 1880	H	0	11.909	-3.768	8.383	H
HETATM 1793	H	0	-10.720	6.788	-6.048	H	HETATM 1881	H	0	11.934	-5.967	6.295	H
HETATM 1794	H	0	-20.794	8.173	0.797	H	HETATM 1882	H	0	12.891	-7.012	0.523	H
HETATM 1795	H	0	-19.782	8.017	-0.475	H	HETATM 1883	H	0	3.030	-0.056	9.085	H
HETATM 1796	H	0	-15.140	8.089	-0.929	H	HETATM 1884	H	0	12.347	-1.182	2.646	H
HETATM 1797	H	0	-13.254	9.936	-1.538	H	HETATM 1885	H	0	11.681	-8.858	-1.179	H
HETATM 1798	H	0	-8.798	13.631	-0.155	H	HETATM 1886	H	0	9.508	-9.845	0.500	H
HETATM 1799	H	0	-9.843	13.063	-2.703	H	HETATM 1887	H	0	7.550	-8.111	-0.160	H
HETATM 1800	H	0	-13.847	12.091	-4.769	H	HETATM 1888	H	0	6.009	-9.446	-1.942	H
HETATM 1801	H	0	-5.481	11.673	-2.587	H	HETATM 1889	H	0	4.006	-10.480	-1.624	H
HETATM 1802	H	0	-5.065	10.978	-4.576	H	HETATM 1890	H	0	5.023	-12.186	-8.541	H
HETATM 1803	H	0	-6.018	4.318	-2.186	H	HETATM 1891	H	0	5.161	-11.748	-10.108	H
HETATM 1804	H	0	-5.789	1.576	-5.420	H	HETATM 1892	H	0	1.372	-8.131	-8.190	H
HETATM 1805	H	0	2.242	14.133	-6.971	H	HETATM 1893	H	0	5.287	-0.919	-1.845	H
HETATM 1806	H	0	1.503	13.287	-8.157	H	HETATM 1894	H	0	5.634	9.075	7.216	H
HETATM 1807	H	0	-1.221	12.008	-4.901	H	HETATM 1895	H	0	3.791	6.777	9.623	H
HETATM 1808	H	0	-3.398	11.315	-5.690	H	HETATM 1896	H	0	3.243	9.373	10.591	H
HETATM 1809	H	0	-1.982	7.368	-10.730	H	HETATM 1897	H	0	6.509	13.167	7.428	H
HETATM 1810	H	0	-1.656	8.020	-12.191	H	HETATM 1898	H	0	6.556	13.827	5.935	H
HETATM 1811	H	0	-5.055	7.046	-12.239	H	HETATM 1899	H	0	-1.928	9.964	5.213	H
HETATM 1812	H	0	-3.928	7.268	-13.400	H	HETATM 1900	H	0	-5.246	-7.687	-7.375	H
HETATM 1813	H	0	-2.042	2.846	-6.537	H	HETATM 1901	H	0	-3.929	-10.996	-9.695	H
HETATM 1814	H	0	-4.357	3.553	-6.870	H	HETATM 1902	H	0	-5.215	-2.386	-14.182	H
HETATM 1815	H	0	-4.877	1.857	-2.843	H	HETATM 1903	H	0	-3.747	-1.515	-14.441	H
HETATM 1816	H	0	13.470	7.268	-9.374	H	HETATM 1904	H	0	-2.396	0.220	-9.206	H
HETATM 1817	H	0	15.543	7.243	-7.527	H	HETATM 1905	H	0	-3.445	-1.883	-7.897	H
HETATM 1818	H	0	16.835	4.989	-7.981	H	HETATM 1906	H	0	-0.185	-6.366	-12.392	H
HETATM 1819	H	0	16.319	4.123	-5.594	H	HETATM 1907	H	0	1.347	-6.233	-11.843	H
HETATM 1820	H	0	13.917	0.431	-4.206	H	HETATM 1908	H	0	-1.988	-3.994	-8.604	H
HETATM 1821	H	0	10.165	0.475	-6.644	H	HETATM 1909	H	0	-1.169	-7.995	-7.062	H
HETATM 1822	H	0	7.667	-1.292	-3.305	H	HETATM 1910	H	0	-10.658	-10.419	-6.488	H
HETATM 1823	H	0	5.261	-4.187	-5.605	H	HETATM 1911	H	0	-10.461	-6.338	-3.824	H
HETATM 1824	H	0	1.334	-4.888	-3.341	H	HETATM 1912	H	0	-12.983	-7.140	-4.751	H
HETATM 1825	H	0	1.403	-2.261	-2.061	H	HETATM 1913	H	0	-11.876	-4.763	-8.108	H
HETATM 1826	H	0	2.952	-1.142	-3.607	H	HETATM 1914	H	0	-9.778	-8.767	-7.233	H
HETATM 1827	H	0	-19.106	9.844	-3.904	H	HETATM 1915	H	0	-13.945	-5.048	-5.869	H
HETATM 1828	H	0	18.823	-0.909	-7.795	H	HETATM 1916	H	0	-16.654	-1.131	-5.050	H
HETATM 1829	H	0	19.719	-0.728	-9.148	H	HETATM 1917	H	0	-15.302	-0.271	-5.365	H
HETATM 1830	H	0	17.597	-2.215	-10.246	H	HETATM 1918	H	0	-17.722	-2.121	-6.753	H
HETATM 1831	H	0	18.829	-1.309	-10.820	H	HETATM 1919	H	0	-17.020	-2.102	-8.227	H
HETATM 1832	H	0	17.405	-5.423	-8.949	H	HETATM 1920	H	0	3.518	13.770	-3.789	H
HETATM 1833	H	0	17.958	-4.186	-9.860	H	HETATM 1921	H	0	0.880	16.034	-3.961	H
HETATM 1834	H	0	14.654	-3.700	-8.465	H	HETATM 1922	H	0	2.214	16.367	-4.842	H
HETATM 1835	H	0	15.238	-3.242	-9.920	H	HETATM 1923	H	0	3.631	15.046	-4.801	H
HETATM 1836	H	0	16.727	-2.831	-6.827	H	HETATM 1924	H	0	-0.717	10.724	-2.507	H
HETATM 1837	H	0	16.753	0.659	-8.184	H	HETATM 1925	H	0	-6.631	8.624	0.562	H
HETATM 1838	H	0	19.039	-4.061	-2.514	H	HETATM 1926	H	0	-0.671	7.981	-3.482	H
HETATM 1839	H	0	13.247	2.835	-8.126	H	HETATM 1927	H	0	3.576	8.552	-2.949	H
HETATM 1840	H	0	11.111	0.458	-11.382	H	HETATM 1928	H	0	1.585	8.465	0.820	H

HETATM 1929 H	0	2.098	9.719	3.229	H	HETATM 1955 H	0	-8.774	1.902	-0.165	H
HETATM 1930 H	0	-1.357	14.357	4.029	H	HETATM 1956 H	0	2.620	2.415	-0.060	H
HETATM 1931 H	0	0.121	15.011	4.261	H	HETATM 1957 H	0	-1.442	0.620	-7.498	H
HETATM 1932 H	0	0.047	11.104	3.845	H	HETATM 1958 H	0	0.916	5.707	-3.581	H
HETATM 1933 H	0	-7.482	5.770	11.377	H	HETATM 1959 H	0	-7.362	-3.264	7.417	H
HETATM 1934 H	0	-7.213	6.061	8.770	H	HETATM 1960 H	0	2.215	-1.948	5.240	H
HETATM 1935 H	0	-10.333	6.995	5.757	H	HETATM 1961 H	0	0.860	-1.004	7.547	H
HETATM 1936 H	0	-7.901	1.996	9.057	H	HETATM 1962 H	0	3.967	1.932	7.487	H
HETATM 1937 H	0	-9.278	-1.744	7.785	H	HETATM 1963 H	0	1.874	3.783	7.256	H
HETATM 1938 H	0	-10.345	2.554	7.493	H	HETATM 1964 H	0	2.278	4.761	9.677	H
HETATM 1939 H	0	-18.493	-7.424	5.671	H	HETATM 1965 H	0	0.060	-5.914	3.984	H
HETATM 1940 H	0	-12.529	-6.084	-0.130	H	HETATM 1966 H	0	0.950	-5.766	6.596	H
HETATM 1941 H	0	-10.468	-7.732	0.762	H	HETATM 1967 H	0	1.899	-7.295	2.774	H
HETATM 1942 H	0	-8.881	-5.744	1.834	H	HETATM 1968 H	0	1.182	-8.681	9.893	H
HETATM 1943 H	0	-10.443	-5.014	3.977	H	HETATM 1969 H	0	2.276	-8.467	8.700	H
HETATM 1944 H	0	-11.266	-4.520	-2.005	H	HETATM 1970 H	0	3.081	-4.146	6.203	H
HETATM 1945 H	0	-13.596	3.660	9.725	H	HETATM 1971 H	0	1.944	-9.745	4.136	H
HETATM 1946 H	0	-12.971	3.968	8.249	H	HETATM 1972 H	0	1.139	-13.925	-3.164	H
HETATM 1947 H	0	-12.173	2.705	5.145	H	HETATM 1973 H	0	-0.177	-13.961	-0.703	H
HETATM 1948 H	0	-10.036	7.112	3.362	H	HETATM 1974 H	0	-2.746	-10.770	1.655	H
HETATM 1949 H	0	-10.582	8.403	2.522	H	HETATM 1975 H	0	-0.965	-10.671	3.583	H
HETATM 1950 H	0	-6.684	3.425	6.317	H	HETATM 1976 H	0	-2.949	-13.670	3.044	H
HETATM 1951 H	0	-10.311	5.259	1.875	H	HETATM 1977 H	0	-4.165	-14.819	4.971	H
HETATM 1952 H	0	-14.370	-0.600	8.545	H	HETATM 1978 H	0	-7.584	-14.141	6.951	H
HETATM 1953 H	0	-12.656	3.519	2.216	H	END					
HETATM 1954 H	0	-8.754	3.560	-2.332	H						

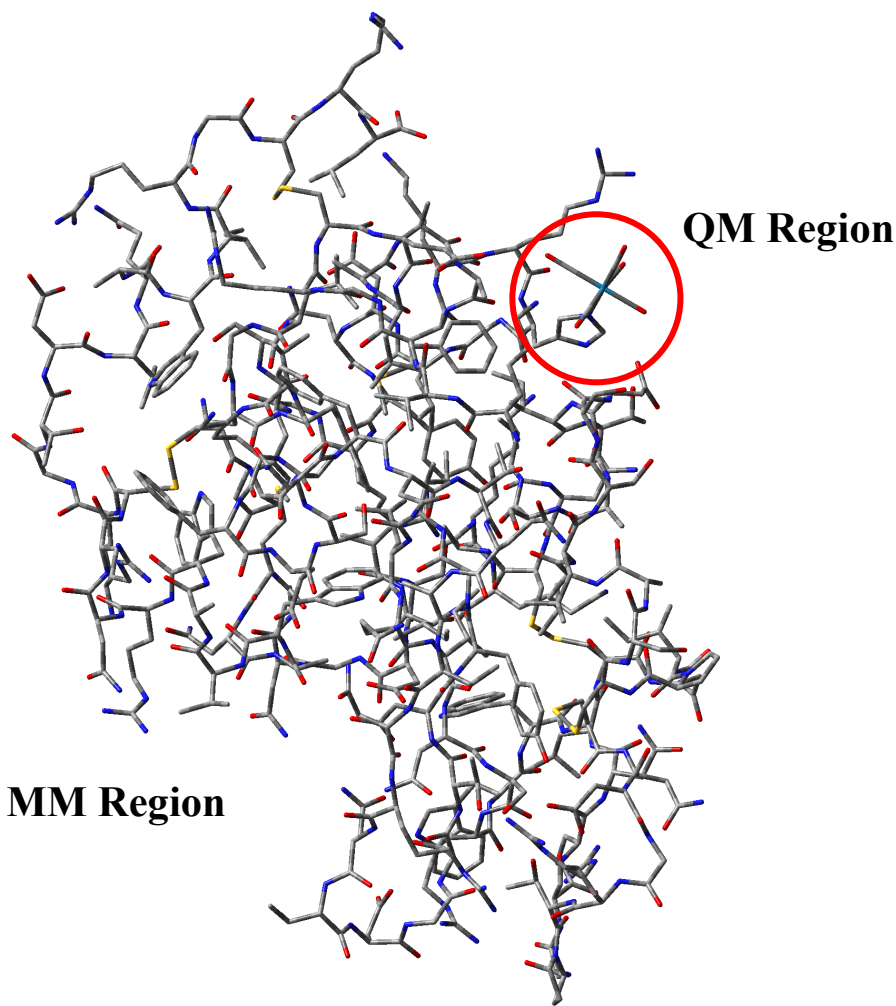


Figure S1. QM/MM optimized structure of Lys1.

Table S2. XYZ coordinates of QM/MM optimized structure of Lys2.

TITLE	Lys2										HETATM	84	O	0	8.074	4.963	4.516	O
REMARK	1 File created by GaussView 5.0.9										HETATM	85	C	0	7.983	3.245	1.667	C
HETATM	1	N	0	0.897	8.759	-10.565				N	HETATM	86	C	0	6.818	2.978	0.741	C
HETATM	2	C	0	2.359	8.749	-10.504				C	HETATM	87	S	0	6.863	1.327	0.070	S
HETATM	3	C	0	2.863	7.325	-10.548				C	HETATM	88	C	0	5.153	1.137	-0.484	C
HETATM	4	O	0	2.363	6.505	-9.741				O	HETATM	89	N	0	10.044	4.989	3.397	N
HETATM	5	C	0	2.847	9.450	-9.223				C	HETATM	90	C	0	10.833	5.194	4.603	C
HETATM	6	C	0	4.383	9.489	-9.123				C	HETATM	91	C	0	10.532	6.551	5.241	C
HETATM	7	C	0	4.831	10.451	-8.019				C	HETATM	92	O	0	10.325	6.623	6.458	O
HETATM	8	C	0	6.347	10.432	-7.825				C	HETATM	93	C	0	12.325	5.074	4.306	C
HETATM	9	N	0	6.718	11.389	-6.787				N	HETATM	94	C	0	13.173	5.219	5.559	C
HETATM	10	N	0	3.800	7.009	-11.449				N	HETATM	95	C	0	14.632	4.929	5.256	C
HETATM	11	C	0	4.524	5.744	-11.433				C	HETATM	96	C	0	15.447	5.042	6.542	C
HETATM	12	C	0	5.874	5.958	-10.791				C	HETATM	97	N	0	16.852	4.559	6.342	N
HETATM	13	O	0	6.742	6.644	-11.387				O	HETATM	98	N	0	10.448	7.592	4.407	N
HETATM	14	C	0	4.638	5.065	-12.856				C	HETATM	99	C	0	8.839	8.953	5.620	C
HETATM	15	C	0	5.411	3.747	-12.798				C	HETATM	100	O	0	8.695	9.605	6.642	O
HETATM	16	C	0	3.240	4.831	-13.488				C	HETATM	101	C	0	11.435	10.773	3.585	C
HETATM	17	N	0	6.042	5.418	-9.576				N	HETATM	102	C	0	12.519	9.988	2.848	C
HETATM	18	C	0	7.344	5.460	-8.872				C	HETATM	103	N	0	13.722	10.822	2.718	N
HETATM	19	C	0	8.357	4.535	-9.476				C	HETATM	104	C	0	14.668	10.269	1.729	C
HETATM	20	O	0	8.033	3.446	-9.967				O	HETATM	105	N	0	14.346	10.799	0.403	N
HETATM	21	C	0	7.207	5.071	-7.396				C	HETATM	106	N	0	16.035	10.664	2.078	N
HETATM	22	C	0	6.674	6.165	-6.538				C	HETATM	107	N	0	7.880	8.174	5.108	N
HETATM	23	C	0	7.549	6.963	-5.788				C	HETATM	108	C	0	6.522	8.104	5.679	C
HETATM	24	C	0	5.290	6.453	-6.504				C	HETATM	109	C	0	6.335	7.018	6.757	C
HETATM	25	C	0	7.075	8.008	-4.970				C	HETATM	110	O	0	5.210	6.727	7.204	O
HETATM	26	C	0	4.809	7.498	-5.711				C	HETATM	111	C	0	5.488	8.016	4.537	C
HETATM	27	C	0	5.688	8.281	-4.940				C	HETATM	112	C	0	5.430	9.358	3.810	C
HETATM	28	N	0	9.625	4.955	-9.407				N	HETATM	113	N	0	4.389	10.273	4.027	N
HETATM	29	C	0	10.710	4.001	-9.537				C	HETATM	114	C	0	6.314	10.035	2.978	C
HETATM	30	C	0	10.847	3.250	-8.222				C	HETATM	115	C	0	4.667	11.438	3.360	C
HETATM	31	O	0	10.389	3.711	-7.184				O	HETATM	116	N	0	5.835	11.325	2.712	N
HETATM	32	N	0	11.457	2.075	-8.286				N	HETATM	117	N	0	7.435	6.422	7.203	N
HETATM	33	C	0	11.646	1.209	-7.134				C	HETATM	118	C	0	7.424	5.563	8.399	C
HETATM	34	C	0	12.344	1.887	-5.925				C	HETATM	119	C	0	7.040	4.100	8.264	C
HETATM	35	O	0	11.822	1.871	-4.795				O	HETATM	120	O	0	6.673	3.453	9.257	O
HETATM	36	C	0	12.382	-0.030	-7.631				C	HETATM	121	N	0	7.128	3.564	7.051	N
HETATM	37	C	0	12.795	-0.989	-6.586				C	HETATM	122	C	0	6.814	2.146	6.826	C
HETATM	38	C	0	13.558	-2.185	-7.238				C	HETATM	123	C	0	7.963	1.176	7.082	C
HETATM	39	N	0	14.855	-1.805	-7.812				N	HETATM	124	O	0	7.757	-0.027	7.235	O
HETATM	40	C	0	15.999	-1.686	-7.126				C	HETATM	125	C	0	6.324	1.924	5.389	C
HETATM	41	N	0	16.062	-1.931	-5.816				N	HETATM	126	C	0	4.838	2.132	5.131	C
HETATM	42	N	0	17.108	-1.345	-7.769				N	HETATM	127	C	0	4.530	1.682	3.693	C
HETATM	43	N	0	13.520	2.499	-6.149				N	HETATM	128	C	0	3.897	1.402	6.166	C
HETATM	44	C	0	14.240	3.139	-5.043				C	HETATM	129	N	0	9.184	1.703	7.101	N
HETATM	45	C	0	13.536	4.420	-4.582				C	HETATM	130	C	0	10.362	0.878	7.275	C
HETATM	46	O	0	13.554	4.741	-3.402				O	HETATM	131	C	0	10.313	0.194	8.651	C
HETATM	47	C	0	15.709	3.433	-5.406				C	HETATM	132	O	0	10.361	0.851	9.704	O
HETATM	48	S	0	16.704	1.952	-5.619				S	HETATM	133	C	0	11.624	1.731	7.085	C
HETATM	49	N	0	12.925	5.138	-5.530				N	HETATM	134	C	0	12.892	0.909	7.094	C
HETATM	50	C	0	12.145	6.323	-5.241				C	HETATM	135	O	0	12.796	-0.349	7.092	O
HETATM	51	C	0	10.987	5.984	-4.281				C	HETATM	136	O	0	14.021	1.552	7.088	O
HETATM	52	O	0	10.773	6.663	-3.265				O	HETATM	137	N	0	10.157	-1.127	8.614	N
HETATM	53	C	0	11.621	6.935	-6.545				C	HETATM	138	C	0	9.874	-1.959	9.787	C
HETATM	54	C	0	10.838	8.186	-6.291				C	HETATM	139	C	0	8.611	-1.750	10.593	C
HETATM	55	C	0	10.158	8.805	-7.508				C	HETATM	140	O	0	8.523	-2.217	11.743	O
HETATM	56	O	0	9.939	8.097	-8.660				O	HETATM	141	C	0	11.073	-2.048	10.714	C
HETATM	57	O	0	9.807	10.007	-7.305				O	HETATM	142	C	0	11.892	-3.249	10.404	C
HETATM	58	N	0	10.284	4.893	-4.559				N	HETATM	143	O	0	11.476	-4.401	10.677	O
HETATM	59	C	0	9.210	4.487	-3.629				C	HETATM	144	N	0	13.030	-3.019	9.754	N
HETATM	60	C	0	9.727	3.979	-2.288				C	HETATM	145	N	0	7.646	-1.035	10.004	N
HETATM	61	O	0	9.126	4.253	-1.242				O	HETATM	146	C	0	6.347	-0.881	10.615	C
HETATM	62	C	0	8.284	3.427	-4.271				C	HETATM	147	C	0	5.746	-2.256	10.864	C
HETATM	63	C	0	7.096	2.983	-3.417				C	HETATM	148	O	0	5.690	-3.135	9.956	O
HETATM	64	C	0	6.179	4.168	-3.057				C	HETATM	149	C	0	5.399	-0.015	9.748	C
HETATM	65	C	0	6.359	1.849	-4.172				C	HETATM	150	C	0	4.159	0.382	10.517	C
HETATM	66	N	0	10.834	3.240	-2.308				N	HETATM	151	C	0	4.151	1.539	11.317	C
HETATM	67	C	0	11.450	2.772	-1.065				C	HETATM	152	C	0	3.028	-0.423	10.519	C
HETATM	68	C	0	11.774	3.965	-0.164				C	HETATM	153	C	0	3.011	1.891	12.074	C
HETATM	69	O	0	11.455	3.965	1.033				O	HETATM	154	C	0	1.885	-0.074	11.268	C
HETATM	70	C	0	12.710	1.923	-1.357				C	HETATM	155	C	0	1.899	1.073	12.059	C
HETATM	71	N	0	12.365	4.994	-0.765				N	HETATM	156	O	0	0.763	1.446	12.776	O
HETATM	72	C	0	12.715	6.212	-0.045				C	HETATM	157	N	0	5.309	-2.480	12.113	N
HETATM	73	C	0	11.487	6.897	0.532				C	HETATM	158	C	0	5.745	-4.946	12.151	C
HETATM	74	O	0	11.458	7.251	1.717				O	HETATM	159	O	0	5.314	-6.069	11.895	O
HETATM	75	C	0	13.479	7.139	-0.958				C	HETATM	160	C	0	1.918	-4.224	13.961	C
HETATM	76	N	0	10.480	7.092	-0.306				N	HETATM	161	N	0	0.800	-3.751	14.793	N
HETATM	77	C	0	9.244	7.722	0.136				C	HETATM	162	C	0	0.653	-2.522	15.305	C
HETATM	78	C	0	8.592	6.906	1.251				C	HETATM	163	N	0	1.969	-1.986	15.680	N
HETATM	79	O	0	8.091	7.475	2.216				O	HETATM	164	N	0	-0.207	-2.587	16.496	N
HETATM	80	C	0	8.304	7.917	-1.022				C	HETATM	165	N	0	7.045	-4.647	12.134	N
HETATM	81	N	0	8.567	5.577	1.096				N	HETATM	166	C	0	8.060	-5.673	11.913	C
HETATM	82	C	0	8.005	4.714	2.124				C	HETATM	167	C	0	8.325	-6.026	10.455	C
HETATM	83	C	0	8.715	4.884	3.457				C	HETATM	168	O	0	9.116	-6.930	10.162	O

HETATM 169	N	0	7.656	-5.319	9.532	N	HETATM 257	C	0	3.096	-8.087	-6.820	C
HETATM 170	C	0	7.850	-5.614	8.119	C	HETATM 258	C	0	4.429	-8.615	-7.281	C
HETATM 171	C	0	8.890	-4.707	7.496	C	HETATM 259	C	0	5.377	-9.024	-6.369	C
HETATM 172	O	0	8.720	-3.484	7.486	O	HETATM 260	C	0	4.748	-8.630	-8.660	C
HETATM 173	C	0	6.514	-5.482	7.387	C	HETATM 261	C	0	6.614	-9.509	-6.791	C
HETATM 174	C	0	5.609	-6.633	7.738	C	HETATM 262	C	0	6.017	-9.086	-9.094	C
HETATM 175	C	0	5.660	-7.832	7.002	C	HETATM 263	C	0	6.939	-9.526	-8.133	C
HETATM 176	C	0	4.684	-6.518	8.807	C	HETATM 264	N	0	1.061	-5.337	-6.377	N
HETATM 177	C	0	4.784	-8.901	7.303	C	HETATM 265	C	0	-0.296	-4.838	-6.270	C
HETATM 178	C	0	3.810	-7.579	9.115	C	HETATM 266	C	0	-0.616	-3.838	-7.386	C
HETATM 179	C	0	3.870	-8.765	8.348	C	HETATM 267	O	0	-1.712	-3.844	-7.951	O
HETATM 180	O	0	3.044	-9.860	8.609	O	HETATM 268	C	0	-0.518	-4.156	-4.912	C
HETATM 181	N	0	10.001	-5.311	7.042	N	HETATM 269	C	0	-0.645	-5.124	-3.718	C
HETATM 182	C	0	11.096	-4.497	6.457	C	HETATM 270	C	0	-1.825	-6.131	-3.806	C
HETATM 183	C	0	10.632	-3.770	5.199	C	HETATM 271	O	0	-2.719	-5.965	-4.689	O
HETATM 184	O	0	9.690	-4.229	4.535	O	HETATM 272	O	0	-1.835	-7.135	-2.949	O
HETATM 185	C	0	12.304	-5.360	6.126	C	HETATM 273	N	0	0.325	-2.917	-7.661	N
HETATM 186	O	0	11.957	-6.351	5.167	O	HETATM 274	C	0	0.036	-1.752	-8.552	C
HETATM 187	N	0	11.309	-2.662	4.871	N	HETATM 275	C	0	1.095	-1.442	-9.595	C
HETATM 188	C	0	11.012	-1.911	3.654	C	HETATM 276	O	0	0.946	-0.480	-10.385	O
HETATM 189	C	0	10.831	-2.751	2.403	C	HETATM 277	C	0	-0.110	-0.489	-7.708	C
HETATM 190	O	0	9.936	-2.475	1.608	O	HETATM 278	O	0	1.144	-0.153	-7.121	O
HETATM 191	C	0	12.118	-0.903	3.325	C	HETATM 279	N	0	2.177	-2.242	-9.596	N
HETATM 192	C	0	11.945	0.614	3.323	C	HETATM 280	C	0	3.356	-1.941	-10.433	C
HETATM 193	C	0	13.116	1.266	2.534	C	HETATM 281	C	0	3.872	-0.527	-10.153	C
HETATM 194	C	0	10.545	1.118	2.905	C	HETATM 282	O	0	4.308	0.181	-11.071	O
HETATM 195	N	0	11.708	-3.719	2.185	N	HETATM 283	C	0	3.094	-2.141	-11.925	C
HETATM 196	C	0	11.594	-4.619	1.033	C	HETATM 284	C	0	4.356	-2.453	-12.689	C
HETATM 197	C	0	10.226	-5.312	0.915	C	HETATM 285	O	0	5.389	-2.824	-12.107	O
HETATM 198	O	0	9.729	-5.502	-0.190	O	HETATM 286	N	0	4.294	-2.281	-14.004	N
HETATM 199	N	0	9.607	-5.664	2.039	N	HETATM 287	N	0	3.747	-0.121	-8.903	N
HETATM 200	C	0	8.247	-6.226	2.020	C	HETATM 288	C	0	4.221	1.178	-8.415	C
HETATM 201	C	0	7.208	-5.306	1.413	C	HETATM 289	C	0	3.427	2.395	-8.946	C
HETATM 202	O	0	6.376	-5.727	0.615	O	HETATM 290	O	0	3.875	3.567	-8.841	O
HETATM 203	C	0	7.799	-6.677	3.424	C	HETATM 291	C	0	5.722	1.353	-8.764	C
HETATM 204	C	0	8.442	-8.004	3.828	C	HETATM 292	C	0	6.643	0.317	-8.207	C
HETATM 205	O	0	8.023	-9.083	3.346	O	HETATM 293	C	0	6.493	-0.200	-6.914	C
HETATM 206	N	0	9.498	-7.937	4.675	N	HETATM 294	C	0	7.768	-0.054	-8.948	C
HETATM 207	N	0	7.304	-4.039	1.790	N	HETATM 295	C	0	7.417	-1.112	-6.393	C
HETATM 208	C	0	6.378	-3.006	1.359	C	HETATM 296	C	0	8.702	-0.919	-8.441	C
HETATM 209	C	0	6.591	-2.686	-0.092	C	HETATM 297	C	0	8.522	-1.492	-7.165	C
HETATM 210	O	0	5.627	-2.477	-0.816	O	HETATM 298	N	0	2.224	2.132	-9.452	N
HETATM 211	C	0	6.574	-1.740	2.232	C	HETATM 299	C	0	1.357	3.167	-10.035	C
HETATM 212	C	0	6.156	-1.980	3.666	C	HETATM 300	C	0	0.313	3.649	-9.022	C
HETATM 213	C	0	6.970	-2.195	4.763	C	HETATM 301	O	0	-0.590	2.885	-8.643	O
HETATM 214	C	0	4.801	-2.111	4.148	C	HETATM 302	C	0	0.696	2.605	-11.280	C
HETATM 215	N	0	6.193	-2.430	5.886	N	HETATM 303	C	0	-0.120	3.620	-12.048	C
HETATM 216	C	0	4.869	-2.388	5.539	C	HETATM 304	O	0	-0.288	4.766	-11.622	O
HETATM 217	C	0	3.538	-1.992	3.536	C	HETATM 305	N	0	-0.573	3.215	-13.229	N
HETATM 218	C	0	3.713	-2.520	6.340	C	HETATM 306	N	0	0.455	4.883	-8.556	N
HETATM 219	C	0	2.392	-2.169	4.327	C	HETATM 307	C	0	-0.479	5.391	-7.561	C
HETATM 220	C	0	2.491	-2.439	5.702	C	HETATM 308	C	0	-1.911	5.429	-8.067	C
HETATM 221	N	0	7.860	-2.614	-0.516	N	HETATM 309	O	0	-2.817	5.389	-7.257	O
HETATM 222	C	0	8.169	-2.374	-1.935	C	HETATM 310	C	0	-0.130	6.815	-7.027	C
HETATM 223	C	0	7.718	-3.526	-2.845	C	HETATM 311	O	0	-0.304	7.776	-8.094	O
HETATM 224	O	0	7.119	-3.284	-3.900	O	HETATM 312	C	0	1.296	6.836	-6.477	C
HETATM 225	C	0	9.682	-1.991	-2.163	C	HETATM 313	N	0	-2.121	5.476	-9.374	N
HETATM 226	C	0	10.018	-1.831	-3.658	C	HETATM 314	C	0	-3.471	5.637	-9.900	C
HETATM 227	C	0	9.997	-0.692	-1.399	C	HETATM 315	C	0	-4.195	4.306	-10.172	C
HETATM 228	N	0	7.980	-4.750	-2.407	N	HETATM 316	O	0	-5.341	4.343	-10.634	O
HETATM 229	C	0	7.522	-5.963	-3.085	C	HETATM 317	C	0	-3.473	6.487	-11.182	C
HETATM 230	C	0	5.979	-5.970	-3.195	C	HETATM 318	C	0	-2.958	7.935	-10.944	C
HETATM 231	O	0	5.450	-6.189	-4.270	O	HETATM 319	C	0	-3.265	8.798	-12.115	C
HETATM 232	C	0	8.036	-7.210	-2.338	C	HETATM 320	O	0	-2.405	9.016	-12.988	O
HETATM 233	S	0	7.646	-8.668	-3.249	S	HETATM 321	N	0	-4.510	9.232	-12.213	N
HETATM 234	N	0	5.288	-5.666	-2.095	N	HETATM 322	N	0	-3.562	3.164	-9.862	N
HETATM 235	C	0	3.814	-5.619	-2.151	C	HETATM 323	C	0	-4.124	1.822	-10.167	C
HETATM 236	C	0	3.350	-4.581	-3.140	C	HETATM 324	C	0	-5.464	1.639	-9.439	C
HETATM 237	O	0	2.429	-4.817	-3.927	O	HETATM 325	O	0	-5.563	1.873	-8.227	O
HETATM 238	C	0	3.203	-5.373	-0.773	C	HETATM 326	C	0	-3.151	0.725	-9.692	C
HETATM 239	N	0	3.951	-3.388	-3.111	N	HETATM 327	N	0	-6.455	1.177	-10.178	N
HETATM 240	C	0	3.520	-2.351	-4.049	C	HETATM 328	C	0	-7.741	0.782	-9.603	C
HETATM 241	C	0	3.782	-2.750	-5.512	C	HETATM 329	C	0	-8.111	-0.563	-10.215	C
HETATM 242	O	0	2.980	-2.460	-6.401	O	HETATM 330	O	0	-7.870	-0.811	-11.409	O
HETATM 243	C	0	4.218	-1.053	-3.728	C	HETATM 331	C	0	-8.885	1.820	-9.896	C
HETATM 244	N	0	4.931	-3.390	-5.772	N	HETATM 332	O	0	-9.097	1.948	-11.306	O
HETATM 245	C	0	5.244	-3.822	-7.129	C	HETATM 333	C	0	-8.567	3.211	-9.311	C
HETATM 246	C	0	4.143	-4.742	-7.694	C	HETATM 334	N	0	-8.715	-1.449	-9.419	N
HETATM 247	O	0	3.627	-4.505	-8.814	O	HETATM 335	C	0	-9.148	-2.733	-9.953	C
HETATM 248	C	0	6.586	-4.573	-7.103	C	HETATM 336	C	0	-10.429	-3.149	-9.245	C
HETATM 249	C	0	6.937	-5.299	-8.357	C	HETATM 337	O	0	-10.461	-3.172	-8.016	O
HETATM 250	C	0	7.295	-4.334	-9.495	C	HETATM 338	C	0	-8.063	-3.811	-9.757	C
HETATM 251	C	0	7.494	-5.115	-10.787	C	HETATM 339	C	0	-6.891	-3.634	-10.714	C
HETATM 252	N	0	7.789	-4.141	-11.881	N	HETATM 340	O	0	-7.026	-3.816	-11.949	O
HETATM 253	N	0	3.737	-5.729	-6.901	N	HETATM 341	N	0	-5.739	-3.257	-10.160	N
HETATM 254	C	0	2.791	-6.716	-7.413	C	HETATM 342	N	0	-11.461	-3.484	-10.034	N
HETATM 255	C	0	1.326	-6.297	-7.251	C	HETATM 343	C	0	-12.767	-3.949	-9.493	C
HETATM 256	O	0	0.457	-6.825	-7.938	O	HETATM 344	C	0	-12.686	-5.400	-9.048	C

HETATM 345	O	0	-12.185	-6.277	-9.800	O	HETATM 433	N	0	-3.363	-1.050	-3.359	N
HETATM 346	C	0	-13.861	-3.828	-10.546	C	HETATM 434	C	0	-4.624	-1.731	-3.704	C
HETATM 347	C	0	-15.297	-3.816	-9.957	C	HETATM 435	C	0	-5.548	-1.947	-2.496	C
HETATM 348	C	0	-15.622	-2.432	-9.478	C	HETATM 436	O	0	-6.054	-3.056	-2.245	O
HETATM 349	N	0	-16.911	-2.332	-8.782	N	HETATM 437	C	0	-4.331	-3.032	-4.445	C
HETATM 350	C	0	-18.025	-1.799	-9.290	C	HETATM 438	C	0	-3.800	-2.729	-5.845	C
HETATM 351	N	0	-18.068	-1.316	-10.534	N	HETATM 439	C	0	-4.873	-2.091	-6.724	C
HETATM 352	N	0	-19.109	-1.724	-8.535	N	HETATM 440	O	0	-5.752	-2.802	-7.239	O
HETATM 353	N	0	-13.197	-5.660	-7.847	N	HETATM 441	N	0	-4.792	-0.773	-6.932	N
HETATM 354	C	0	-13.321	-7.007	-7.300	C	HETATM 442	N	0	-5.785	-0.848	-1.803	N
HETATM 355	C	0	-14.652	-7.645	-7.689	C	HETATM 443	C	0	-6.615	-0.863	-0.593	C
HETATM 356	O	0	-15.615	-6.949	-7.986	O	HETATM 444	C	0	-8.084	-0.927	-0.974	C
HETATM 357	C	0	-13.187	-6.956	-5.767	C	HETATM 445	O	0	-8.530	-0.173	-1.842	O
HETATM 358	C	0	-11.885	-6.336	-5.314	C	HETATM 446	C	0	-6.241	0.351	0.255	C
HETATM 359	O	0	-11.852	-5.457	-4.429	O	HETATM 447	C	0	-4.800	0.134	0.830	C
HETATM 360	N	0	-10.801	-6.745	-5.958	N	HETATM 448	C	0	-7.266	0.610	1.371	C
HETATM 361	N	0	-14.689	-8.975	-7.700	N	HETATM 449	C	0	-4.263	1.399	1.557	C
HETATM 362	C	0	-15.907	-9.715	-8.077	C	HETATM 450	N	0	-8.805	-1.859	-0.331	N
HETATM 363	C	0	-17.125	-9.371	-7.212	C	HETATM 451	C	0	-10.146	-2.324	-0.725	C
HETATM 364	O	0	-18.264	-9.363	-7.697	O	HETATM 452	C	0	-11.280	-1.466	-0.126	C
HETATM 365	C	0	-15.667	-11.259	-8.167	C	HETATM 453	O	0	-11.296	-1.246	1.103	O
HETATM 366	O	0	-15.134	-11.743	-6.929	O	HETATM 454	C	0	-10.276	-3.807	-0.304	C
HETATM 367	C	0	-14.690	-11.538	-9.287	C	HETATM 455	C	0	-11.440	-4.542	-0.973	C
HETATM 368	N	0	-16.869	-9.015	-5.962	N	HETATM 456	O	0	-12.369	-3.922	-1.474	O
HETATM 369	C	0	-17.947	-8.696	-5.029	C	HETATM 457	N	0	-11.378	-5.900	-0.988	N
HETATM 370	C	0	-18.509	-7.275	-5.184	C	HETATM 458	N	0	-12.203	-0.977	-0.966	N
HETATM 371	O	0	-19.425	-6.908	-4.445	O	HETATM 459	C	0	-13.357	-0.198	-0.499	C
HETATM 372	C	0	-17.504	-8.974	-3.592	C	HETATM 460	C	0	-14.312	-1.030	0.389	C
HETATM 373	C	0	-16.450	-7.993	-3.082	C	HETATM 461	O	0	-15.164	-0.444	1.024	O
HETATM 374	O	0	-16.043	-7.050	-3.795	O	HETATM 462	C	0	-14.159	0.377	-1.678	C
HETATM 375	O	0	-16.006	-8.160	-1.871	O	HETATM 463	O	0	-14.681	-0.709	-2.465	O
HETATM 376	N	0	-17.928	-6.483	-6.101	N	HETATM 464	N	0	-14.164	-2.353	0.407	N
HETATM 377	C	0	-18.365	-5.124	-6.374	C	HETATM 465	C	0	-14.993	-3.282	1.228	C
HETATM 378	C	0	-17.548	-4.058	-5.642	C	HETATM 466	C	0	-14.905	-2.861	2.706	C
HETATM 379	O	0	-17.700	-2.871	-5.909	O	HETATM 467	O	0	-15.906	-2.877	3.435	O
HETATM 380	N	0	-16.653	-4.482	-4.748	N	HETATM 468	C	0	-14.466	-4.717	1.041	C
HETATM 381	C	0	-15.762	-3.510	-4.116	C	HETATM 469	C	0	-15.243	-5.853	1.754	C
HETATM 382	C	0	-14.690	-3.169	-5.171	C	HETATM 470	C	0	-16.256	-6.472	0.824	C
HETATM 383	O	0	-14.598	-3.831	-6.208	O	HETATM 471	N	0	-17.568	-5.880	1.055	N
HETATM 384	C	0	-15.130	-4.061	-2.840	C	HETATM 472	C	0	-18.497	-5.646	0.126	C
HETATM 385	O	0	-14.321	-5.194	-3.122	O	HETATM 473	N	0	-18.292	-5.926	-1.164	N
HETATM 386	N	0	-13.896	-2.141	-4.878	N	HETATM 474	N	0	-19.642	-5.089	0.507	N
HETATM 387	C	0	-12.745	-1.764	-5.748	C	HETATM 475	N	0	-13.712	-2.454	3.129	N
HETATM 388	C	0	-11.479	-1.584	-4.918	C	HETATM 476	C	0	-13.435	-2.147	4.534	C
HETATM 389	O	0	-11.546	-1.153	-3.767	O	HETATM 477	C	0	-12.851	-0.785	4.828	C
HETATM 390	C	0	-13.109	-0.486	-6.517	C	HETATM 478	O	0	-13.064	-0.209	5.897	O
HETATM 391	O	0	-14.323	-0.728	-7.247	O	HETATM 479	C	0	-12.442	-3.181	5.087	C
HETATM 392	C	0	-12.027	-0.058	-7.527	C	HETATM 480	C	0	-13.069	-4.526	5.178	C
HETATM 393	N	0	-10.317	-1.932	-5.509	N	HETATM 481	C	0	-12.815	-5.605	4.385	C
HETATM 394	C	0	-8.988	-1.746	-4.875	C	HETATM 482	C	0	-14.110	-4.912	6.082	C
HETATM 395	C	0	-8.327	-0.489	-5.459	C	HETATM 483	N	0	-13.625	-6.656	4.757	N
HETATM 396	O	0	-8.379	-0.259	-6.682	O	HETATM 484	C	0	-14.428	-6.254	5.797	C
HETATM 397	C	0	-8.075	-2.980	-5.109	C	HETATM 485	C	0	-14.809	-4.242	7.110	C
HETATM 398	C	0	-8.484	-4.223	-4.281	C	HETATM 486	C	0	-15.411	-6.960	6.514	C
HETATM 399	O	0	-9.409	-4.147	-3.453	O	HETATM 487	C	0	-15.794	-4.944	7.831	C
HETATM 400	O	0	-7.786	-5.329	-4.461	O	HETATM 488	C	0	-16.083	-6.288	7.521	C
HETATM 401	N	0	-7.789	0.358	-4.576	N	HETATM 489	N	0	-12.048	-0.282	3.893	N
HETATM 402	C	0	-7.224	1.638	-4.968	C	HETATM 490	C	0	-11.064	0.718	4.266	C
HETATM 403	C	0	-5.752	1.822	-4.621	C	HETATM 491	C	0	-11.284	2.136	3.798	C
HETATM 404	O	0	-5.342	1.552	-3.494	O	HETATM 492	O	0	-10.818	3.067	4.449	O
HETATM 405	C	0	-8.011	2.772	-4.282	C	HETATM 493	C	0	-9.646	0.246	3.866	C
HETATM 406	C	0	-9.449	2.822	-4.715	C	HETATM 494	C	0	-9.294	-1.092	4.439	C
HETATM 407	C	0	-9.859	3.664	-5.766	C	HETATM 495	C	0	-9.197	-2.255	3.763	C
HETATM 408	C	0	-10.417	1.995	-4.103	C	HETATM 496	C	0	-9.048	-1.395	5.808	C
HETATM 409	C	0	-11.202	3.694	-6.183	C	HETATM 497	N	0	-8.881	-3.284	4.618	N
HETATM 410	C	0	-11.757	2.021	-4.505	C	HETATM 498	C	0	-8.821	-2.794	5.889	C
HETATM 411	C	0	-12.130	2.863	-5.529	C	HETATM 499	C	0	-9.006	-0.624	6.974	C
HETATM 412	O	0	-13.435	2.903	-5.931	O	HETATM 500	C	0	-8.531	-3.453	7.104	C
HETATM 413	N	0	-4.990	2.319	-5.596	N	HETATM 501	C	0	-8.717	-1.276	8.191	C
HETATM 414	C	0	-3.665	2.904	-5.285	C	HETATM 502	C	0	-8.478	-2.684	8.225	C
HETATM 415	C	0	-2.507	1.919	-5.219	C	HETATM 503	N	0	-11.995	2.323	2.696	N
HETATM 416	O	0	-2.629	0.739	-5.566	O	HETATM 504	C	0	-12.189	3.676	2.194	C
HETATM 417	N	0	-1.359	2.444	-4.809	N	HETATM 505	C	0	-13.600	3.764	1.640	C
HETATM 418	C	0	-0.111	1.681	-4.757	C	HETATM 506	O	0	-14.220	2.718	1.350	O
HETATM 419	C	0	-0.184	0.358	-3.990	C	HETATM 507	C	0	-11.115	4.070	1.154	C
HETATM 420	O	0	0.455	-0.621	-4.381	O	HETATM 508	S	0	-11.083	3.018	-0.355	S
HETATM 421	C	0	1.130	2.476	-4.210	C	HETATM 509	N	0	-14.109	4.990	1.519	N
HETATM 422	C	0	0.854	3.108	-2.836	C	HETATM 510	C	0	-15.412	5.184	0.908	C
HETATM 423	C	0	1.720	3.348	-5.307	C	HETATM 511	C	0	-15.334	5.572	-0.563	C
HETATM 424	C	0	2.170	3.439	-2.063	C	HETATM 512	O	0	-14.651	6.554	-0.899	O
HETATM 425	N	0	-0.999	0.323	-2.935	N	HETATM 513	C	0	-16.214	6.240	1.641	C
HETATM 426	C	0	-1.208	-0.884	-2.196	C	HETATM 514	C	0	-17.566	6.439	0.978	C
HETATM 427	C	0	-2.609	-1.495	-2.343	C	HETATM 515	O	0	-18.286	5.464	0.760	O
HETATM 428	O	0	-2.996	-2.370	-1.564	O	HETATM 516	N	0	-17.862	7.642	0.572	N
HETATM 429	C	0	-0.781	-0.705	-0.718	C	HETATM 517	N	0	-15.982	4.782	-1.422	N
HETATM 430	C	0	0.751	-0.563	-0.496	C	HETATM 518	C	0	-16.103	5.145	-2.833	C
HETATM 431	C	0	1.034	-0.001	0.928	C	HETATM 519	C	0	-17.561	5.366	-3.259	C
HETATM 432	C	0	1.498	-1.907	-0.754	C	HETATM 520	O	0	-17.808	5.652	-4.416	O

HETATM 521	C	0	-15.361	4.161	-3.761	C	HETATM 609	C	0	-9.460	8.383	3.331	C
HETATM 522	C	0	-16.008	2.771	-3.827	C	HETATM 610	C	0	-9.257	6.856	3.297	C
HETATM 523	O	0	-17.095	2.548	-3.253	O	HETATM 611	C	0	-8.498	9.171	4.250	C
HETATM 524	O	0	-15.372	1.846	-4.503	O	HETATM 612	C	0	-7.895	6.382	2.727	C
HETATM 525	N	0	-18.490	5.240	-2.313	N	HETATM 613	N	0	-11.938	9.251	1.467	N
HETATM 526	C	0	-19.891	5.551	-2.596	C	HETATM 614	C	0	-12.453	8.849	0.153	C
HETATM 527	C	0	-20.646	4.529	-3.429	C	HETATM 615	C	0	-11.391	7.996	-0.538	C
HETATM 528	O	0	-21.803	4.780	-3.806	O	HETATM 616	O	0	-10.185	8.286	-0.439	O
HETATM 529	N	0	-19.999	3.424	-3.773	N	HETATM 617	C	0	-12.639	10.171	-0.610	C
HETATM 530	C	0	-20.603	2.376	-4.593	C	HETATM 618	C	0	-11.878	11.215	0.165	C
HETATM 531	C	0	-20.292	0.949	-4.126	C	HETATM 619	C	0	-11.493	10.661	1.511	C
HETATM 532	O	0	-20.340	-0.012	-4.916	O	HETATM 620	N	0	-11.824	6.923	-1.202	N
HETATM 533	C	0	-20.236	2.558	-6.092	C	HETATM 621	C	0	-10.870	6.053	-1.883	C
HETATM 534	C	0	-18.757	2.331	-6.386	C	HETATM 622	C	0	-10.016	6.849	-2.887	C
HETATM 535	C	0	-18.564	2.108	-7.873	C	HETATM 623	O	0	-8.867	6.497	-3.142	O
HETATM 536	N	0	-17.281	1.474	-8.128	N	HETATM 624	C	0	-11.622	4.917	-2.576	C
HETATM 537	C	0	-16.672	1.462	-9.318	C	HETATM 625	S	0	-12.542	3.824	-1.481	S
HETATM 538	N	0	-17.222	2.121	-10.331	N	HETATM 626	N	0	-10.591	7.883	-3.492	N
HETATM 539	N	0	-15.489	0.829	-9.497	N	HETATM 627	C	0	-9.828	8.767	-4.397	C
HETATM 540	N	0	-19.957	0.781	-2.853	N	HETATM 628	C	0	-8.512	9.287	-3.779	C
HETATM 541	C	0	-19.745	-0.551	-2.325	C	HETATM 629	O	0	-7.518	9.495	-4.483	O
HETATM 542	C	0	-20.696	-0.825	-1.163	C	HETATM 630	C	0	-10.709	9.900	-4.958	C
HETATM 543	O	0	-20.371	-0.518	-0.009	O	HETATM 631	O	0	-11.148	10.774	-3.912	O
HETATM 544	C	0	-18.274	-0.753	-1.855	C	HETATM 632	N	0	-8.503	9.503	-2.465	N
HETATM 545	O	0	-17.408	-0.277	-2.903	O	HETATM 633	C	0	-7.280	9.943	-1.759	C
HETATM 546	C	0	-18.000	-2.202	-1.563	C	HETATM 634	C	0	-6.130	8.972	-1.902	C
HETATM 547	N	0	-21.867	-1.390	-1.471	N	HETATM 635	O	0	-4.954	9.369	-1.783	O
HETATM 548	C	0	-22.868	-1.612	-0.416	C	HETATM 636	C	0	-7.564	10.169	-0.286	C
HETATM 549	C	0	-22.342	-2.350	0.797	C	HETATM 637	N	0	-6.470	7.701	-2.120	N
HETATM 550	O	0	-21.528	-3.285	0.677	O	HETATM 638	C	0	-5.483	6.644	-2.276	C
HETATM 551	C	0	-23.933	-2.433	-1.143	C	HETATM 639	C	0	-4.827	6.653	-3.669	C
HETATM 552	C	0	-23.934	-1.788	-2.574	C	HETATM 640	O	0	-3.973	5.802	-3.965	O
HETATM 553	C	0	-22.422	-1.625	-2.821	C	HETATM 641	C	0	-6.137	5.300	-1.986	C
HETATM 554	N	0	-22.785	-1.915	1.975	N	HETATM 642	C	0	-6.740	5.220	-0.590	C
HETATM 555	C	0	-22.592	-2.693	3.197	C	HETATM 643	C	0	-7.469	3.875	-0.487	C
HETATM 556	C	0	-21.171	-2.572	3.643	C	HETATM 644	C	0	-5.605	5.319	0.466	C
HETATM 557	O	0	-20.712	-3.319	4.505	O	HETATM 645	N	0	-5.217	7.606	-4.521	N
HETATM 558	N	0	-20.497	-1.598	3.040	N	HETATM 646	C	0	-4.661	7.642	-5.889	C
HETATM 559	C	0	-19.085	-1.357	3.136	C	HETATM 647	C	0	-3.696	8.794	-6.116	C
HETATM 560	C	0	-18.743	-0.561	4.390	C	HETATM 648	O	0	-3.186	8.962	-7.223	O
HETATM 561	O	0	-19.556	0.221	4.890	O	HETATM 649	C	0	-5.811	7.745	-6.899	C
HETATM 562	C	0	-18.675	-0.547	1.901	C	HETATM 650	C	0	-6.837	6.612	-6.825	C
HETATM 563	O	0	-17.385	-0.045	2.021	O	HETATM 651	C	0	-7.783	6.790	-8.016	C
HETATM 564	N	0	-17.525	-0.753	4.892	N	HETATM 652	C	0	-6.209	5.215	-6.859	C
HETATM 565	C	0	-16.992	0.192	5.868	C	HETATM 653	N	0	-3.446	9.566	-5.057	N
HETATM 566	C	0	-15.940	1.118	5.243	C	HETATM 654	C	0	-2.667	10.807	-5.151	C
HETATM 567	O	0	-15.534	0.935	4.065	O	HETATM 655	C	0	-1.198	10.515	-5.370	C
HETATM 568	C	0	-16.389	-0.546	7.070	C	HETATM 656	O	0	-0.676	9.496	-4.841	O
HETATM 569	C	0	-17.350	-1.553	7.709	C	HETATM 657	C	0	-2.867	11.653	-3.885	C
HETATM 570	C	0	-18.444	-0.836	8.539	C	HETATM 658	O	0	-2.241	12.897	-4.027	O
HETATM 571	N	0	-17.893	-0.281	9.777	N	HETATM 659	N	0	-0.433	11.399	-6.066	N
HETATM 572	C	0	-17.746	-0.961	10.918	C	HETATM 660	C	0	1.025	11.272	-6.229	C
HETATM 573	N	0	-18.140	-2.228	11.006	N	HETATM 661	C	0	1.734	11.314	-4.897	C
HETATM 574	N	0	-17.217	-0.373	11.988	N	HETATM 662	O	0	2.805	10.666	-4.744	O
HETATM 575	N	0	-15.531	2.101	6.048	N	HETATM 663	C	0	1.560	12.382	-7.150	C
HETATM 576	C	0	-14.589	3.157	5.678	C	HETATM 664	O	0	1.248	13.657	-6.651	O
HETATM 577	C	0	-13.686	3.405	6.884	C	HETATM 665	N	0	1.255	12.180	-3.860	N
HETATM 578	O	0	-13.655	4.524	7.449	O	HETATM 666	C	0	1.647	12.055	-2.452	C
HETATM 579	C	0	-15.362	4.421	5.285	C	HETATM 667	C	0	1.132	10.744	-1.893	C
HETATM 580	C	0	-14.445	5.639	4.958	C	HETATM 668	O	0	-0.097	10.480	-1.996	O
HETATM 581	O	0	-14.922	6.771	4.818	O	HETATM 669	C	0	1.085	13.268	-1.678	C
HETATM 582	N	0	-13.157	5.392	4.807	N	HETATM 670	C	0	1.290	13.187	-0.195	C
HETATM 583	N	0	-12.929	2.363	7.229	N	HETATM 671	O	0	0.291	13.251	0.566	O
HETATM 584	C	0	-12.160	2.287	8.473	C	HETATM 672	O	0	2.565	13.109	0.360	O
HETATM 585	C	0	-10.944	3.211	8.495	C	HETATM 673	N	0	1.972	9.875	-1.255	N
HETATM 586	O	0	-10.468	3.588	9.564	O	HETATM 674	C	0	1.529	8.550	-0.762	C
HETATM 587	C	0	-11.750	0.842	8.730	C	HETATM 675	C	0	1.040	8.575	0.684	C
HETATM 588	C	0	-12.502	-0.079	9.710	C	HETATM 676	O	0	0.749	7.519	1.214	O
HETATM 589	C	0	-13.827	0.501	10.202	C	HETATM 677	C	0	2.654	7.476	-0.922	C
HETATM 590	C	0	-12.665	-1.461	9.159	C	HETATM 678	C	0	3.854	7.739	0.025	C
HETATM 591	N	0	-10.469	3.615	7.320	N	HETATM 679	C	0	3.096	7.386	-2.416	C
HETATM 592	C	0	-9.423	4.637	7.234	C	HETATM 680	C	0	4.857	6.622	0.097	C
HETATM 593	C	0	-9.933	6.076	7.199	C	HETATM 681	N	0	0.959	9.758	1.314	N
HETATM 594	O	0	-9.127	7.039	7.211	O	HETATM 682	C	0	0.544	9.834	2.742	C
HETATM 595	C	0	-8.507	4.345	6.032	C	HETATM 683	C	0	-0.729	9.028	3.086	C
HETATM 596	S	0	-7.523	2.867	6.328	S	HETATM 684	O	0	-0.716	8.218	3.998	O
HETATM 597	N	0	-11.259	6.229	7.160	N	HETATM 685	C	0	0.410	11.309	3.196	C
HETATM 598	C	0	-11.938	7.526	7.104	C	HETATM 686	O	0	1.613	11.981	2.940	O
HETATM 599	C	0	-11.462	8.460	6.010	C	HETATM 687	C	0	0.081	11.425	4.689	C
HETATM 600	O	0	-11.081	9.586	6.265	O	HETATM 688	N	0	-1.805	9.260	2.340	N
HETATM 601	C	0	-11.884	8.228	8.482	C	HETATM 689	C	0	-3.073	8.573	2.605	C
HETATM 602	C	0	-12.498	7.372	9.566	C	HETATM 690	C	0	-2.927	7.053	2.512	C
HETATM 603	O	0	-13.723	7.185	9.587	O	HETATM 691	O	0	-3.389	6.318	3.402	O
HETATM 604	N	0	-11.663	6.808	10.445	N	HETATM 692	C	0	-4.196	9.108	1.670	C
HETATM 605	N	0	-11.458	7.966	4.773	N	HETATM 693	N	0	-2.217	6.576	1.487	N
HETATM 606	C	0	-10.956	8.724	3.646	C	HETATM 694	C	0	-2.068	5.137	1.295	C
HETATM 607	C	0	-11.753	8.310	2.416	C	HETATM 695	C	0	-1.251	4.546	2.439	C
HETATM 608	O	0	-12.173	7.136	2.321	O	HETATM 696	O	0	-1.601	3.509	2.984	O

HETATM 697	C	0	-1.442	4.797	-0.058	C	HETATM 785	C	0	-0.081	-8.619	9.170	C
HETATM 698	O	0	-2.421	4.957	-1.080	O	HETATM 786	C	0	-0.245	-8.338	7.678	C
HETATM 699	N	0	-0.186	5.247	2.812	N	HETATM 787	O	0	-1.325	-7.912	7.208	O
HETATM 700	C	0	0.674	4.784	3.900	C	HETATM 788	N	0	0.794	-8.637	6.916	N
HETATM 701	C	0	-0.097	4.736	5.215	C	HETATM 789	C	0	0.739	-8.307	5.474	C
HETATM 702	O	0	-0.056	3.707	5.925	O	HETATM 790	C	0	-0.048	-9.322	4.626	C
HETATM 703	C	0	1.966	5.666	4.052	C	HETATM 791	O	0	-0.191	-9.143	3.404	O
HETATM 704	C	0	2.704	5.284	5.343	C	HETATM 792	C	0	2.139	-8.055	4.904	C
HETATM 705	C	0	2.866	5.405	2.872	C	HETATM 793	C	0	2.745	-6.750	5.398	C
HETATM 706	N	0	-0.801	5.826	5.542	N	HETATM 794	S	0	4.220	-6.217	4.422	S
HETATM 707	C	0	-1.516	5.870	6.814	C	HETATM 795	C	0	3.433	-5.663	2.883	C
HETATM 708	C	0	-2.555	4.753	6.900	C	HETATM 796	N	0	-0.581	-10.362	5.275	N
HETATM 709	O	0	-2.738	4.144	7.970	O	HETATM 797	C	0	-1.392	-11.366	4.602	C
HETATM 710	C	0	-2.200	7.223	7.037	C	HETATM 798	C	0	-2.700	-10.750	4.095	C
HETATM 711	C	0	-1.206	8.340	7.259	C	HETATM 799	O	0	-3.368	-11.339	3.272	O
HETATM 712	O	0	-0.009	8.094	7.411	O	HETATM 800	C	0	-1.681	-12.551	5.527	C
HETATM 713	N	0	-1.690	9.578	7.230	N	HETATM 801	C	0	-0.434	-13.359	5.844	C
HETATM 714	N	0	-3.227	4.499	5.768	N	HETATM 802	O	0	0.169	-13.980	4.953	O
HETATM 715	C	0	-4.267	3.484	5.774	C	HETATM 803	N	0	-0.079	-13.417	7.136	N
HETATM 716	C	0	-3.650	2.071	5.844	C	HETATM 804	N	0	-2.988	-9.551	4.581	N
HETATM 717	O	0	-4.136	1.168	6.567	O	HETATM 805	C	0	-4.075	-8.728	4.063	C
HETATM 718	C	0	-5.201	3.695	4.561	C	HETATM 806	C	0	-3.925	-8.437	2.581	C
HETATM 719	S	0	-6.615	2.537	4.537	S	HETATM 807	O	0	-4.925	-8.198	1.899	O
HETATM 720	N	0	-2.550	1.880	5.108	N	HETATM 808	C	0	-4.216	-7.435	4.866	C
HETATM 721	C	0	-1.826	0.607	5.164	C	HETATM 809	N	0	-2.687	-8.422	2.078	N
HETATM 722	C	0	-1.300	0.267	6.577	C	HETATM 810	C	0	-2.417	-8.202	0.642	C
HETATM 723	O	0	-1.316	-0.891	6.978	O	HETATM 811	C	0	-2.155	-9.547	-0.010	C
HETATM 724	C	0	-0.699	0.583	4.127	C	HETATM 812	O	0	-1.083	-10.160	0.169	O
HETATM 725	N	0	-0.909	1.281	7.353	N	HETATM 813	C	0	-1.236	-7.234	0.444	C
HETATM 726	C	0	-0.539	1.049	8.768	C	HETATM 814	C	0	-1.577	-5.830	0.836	C
HETATM 727	C	0	-1.702	0.453	9.574	C	HETATM 815	C	0	-2.239	-4.900	0.060	C
HETATM 728	O	0	-1.501	-0.423	10.407	O	HETATM 816	C	0	-1.343	-5.200	2.099	C
HETATM 729	C	0	-0.059	2.359	9.403	C	HETATM 817	N	0	-2.388	-3.712	0.761	N
HETATM 730	C	0	1.318	2.803	8.886	C	HETATM 818	C	0	-1.883	-3.888	2.023	C
HETATM 731	C	0	1.711	4.231	9.360	C	HETATM 819	C	0	-0.754	-5.625	3.312	C
HETATM 732	C	0	3.109	4.566	8.867	C	HETATM 820	C	0	-1.801	-2.977	3.071	C
HETATM 733	N	0	3.599	5.919	9.361	N	HETATM 821	C	0	-0.684	-4.690	4.385	C
HETATM 734	N	0	-2.934	0.946	9.334	N	HETATM 822	C	0	-1.203	-3.392	4.248	C
HETATM 735	C	0	-4.111	0.374	9.983	C	HETATM 823	N	0	-3.126	-10.033	-0.763	N
HETATM 736	C	0	-4.398	-1.069	9.543	C	HETATM 824	C	0	-2.996	-11.363	-1.336	C
HETATM 737	O	0	-4.675	-1.948	10.365	O	HETATM 825	C	0	-1.741	-11.493	-2.220	C
HETATM 738	C	0	-5.350	1.218	9.696	C	HETATM 826	O	0	-1.067	-12.514	-2.130	O
HETATM 739	C	0	-5.338	2.539	10.345	C	HETATM 827	C	0	-4.283	-11.862	-2.044	C
HETATM 740	C	0	-6.564	3.376	9.898	C	HETATM 828	C	0	-4.689	-10.943	-3.165	C
HETATM 741	C	0	-6.326	4.846	10.287	C	HETATM 829	C	0	-4.105	-13.312	-2.560	C
HETATM 742	N	0	-6.207	4.917	11.787	N	HETATM 830	N	0	-1.433	-10.468	-3.016	N
HETATM 743	N	0	-4.301	-1.316	8.243	N	HETATM 831	C	0	-0.219	-10.489	-3.844	C
HETATM 744	C	0	-4.546	-2.641	7.682	C	HETATM 832	C	0	1.030	-10.536	-2.967	C
HETATM 745	C	0	-3.568	-3.687	8.265	C	HETATM 833	O	0	2.003	-11.224	-3.333	O
HETATM 746	O	0	-3.978	-4.737	8.735	O	HETATM 834	C	0	-0.151	-9.362	-4.822	C
HETATM 747	C	0	-4.435	-2.626	6.133	C	HETATM 835	N	0	1.038	-9.832	-1.824	N
HETATM 748	C	0	-5.553	-1.768	5.523	C	HETATM 836	C	0	2.175	-10.060	-0.898	C
HETATM 749	C	0	-4.544	-4.054	5.572	C	HETATM 837	C	0	2.274	-11.521	-0.422	C
HETATM 750	C	0	-5.313	-1.286	4.103	C	HETATM 838	O	0	3.371	-12.120	-0.443	O
HETATM 751	N	0	-2.277	-3.369	8.210	N	HETATM 839	C	0	2.184	-9.083	0.301	C
HETATM 752	C	0	-1.251	-4.272	8.678	C	HETATM 840	C	0	3.328	-9.358	1.264	C
HETATM 753	C	0	-1.284	-4.503	10.185	C	HETATM 841	C	0	4.566	-8.797	1.221	C
HETATM 754	O	0	-0.698	-5.480	10.668	O	HETATM 842	C	0	3.320	-10.228	2.414	C
HETATM 755	C	0	0.141	-3.817	8.177	C	HETATM 843	N	0	5.346	-9.283	2.264	N
HETATM 756	C	0	0.684	-2.619	9.004	C	HETATM 844	C	0	4.618	-10.181	2.988	C
HETATM 757	C	0	1.121	-5.017	8.113	C	HETATM 845	C	0	2.374	-11.092	2.966	C
HETATM 758	N	0	-1.991	-3.612	10.899	N	HETATM 846	C	0	4.974	-10.917	4.149	C
HETATM 759	C	0	-2.169	-3.716	12.355	C	HETATM 847	C	0	2.715	-11.811	4.123	C
HETATM 760	C	0	-3.383	-4.515	12.767	C	HETATM 848	C	0	4.017	-11.743	4.678	C
HETATM 761	O	0	-3.563	-4.804	13.966	O	HETATM 849	N	0	1.158	-12.114	-0.004	N
HETATM 762	C	0	-2.238	-2.339	13.005	C	HETATM 850	C	0	1.209	-13.518	0.464	C
HETATM 763	O	0	-1.053	-1.609	12.781	O	HETATM 851	C	0	1.755	-14.456	-0.620	C
HETATM 764	N	0	-4.225	-4.887	11.816	N	HETATM 852	O	0	2.619	-15.283	-0.340	O
HETATM 765	C	0	-5.516	-5.472	12.190	C	HETATM 853	C	0	-0.163	-14.006	0.959	C
HETATM 766	C	0	-5.512	-6.957	12.568	C	HETATM 854	C	0	-0.118	-15.383	1.628	C
HETATM 767	O	0	-6.573	-7.546	12.794	O	HETATM 855	C	0	-1.482	-15.816	2.240	C
HETATM 768	C	0	-6.601	-5.134	11.170	C	HETATM 856	N	0	-2.637	-15.464	1.406	N
HETATM 769	C	0	-6.540	-5.990	9.926	C	HETATM 857	C	0	-3.068	-16.159	0.350	C
HETATM 770	O	0	-5.789	-7.063	9.903	O	HETATM 858	N	0	-2.439	-17.263	-0.045	N
HETATM 771	O	0	-7.241	-5.630	8.950	O	HETATM 859	N	0	-4.129	-15.735	-0.325	N
HETATM 772	N	0	-4.329	-7.568	12.660	N	HETATM 860	N	0	1.282	-14.264	-1.845	N
HETATM 773	C	0	-4.246	-8.962	13.129	C	HETATM 861	C	0	1.533	-15.207	-2.940	C
HETATM 774	C	0	-3.573	-9.962	12.199	C	HETATM 862	C	0	2.831	-14.933	-3.655	C
HETATM 775	O	0	-2.910	-10.887	12.670	O	HETATM 863	O	0	3.380	-15.833	-4.295	O
HETATM 776	N	0	-3.681	-9.764	10.884	N	HETATM 864	C	0	0.368	-15.175	-3.956	C
HETATM 777	C	0	-3.098	-10.730	9.956	C	HETATM 865	C	0	-0.892	-15.822	-3.416	C
HETATM 778	C	0	-1.846	-10.243	9.244	C	HETATM 866	O	0	-0.816	-16.740	-2.590	O
HETATM 779	O	0	-1.374	-10.888	8.304	O	HETATM 867	N	0	-2.053	-15.347	-3.876	N
HETATM 780	C	0	-4.128	-11.232	8.943	C	HETATM 868	N	0	3.336	-13.696	-3.578	N
HETATM 781	C	0	-5.216	-12.051	9.602	C	HETATM 869	C	0	4.506	-13.329	-4.399	C
HETATM 782	O	0	-4.932	-12.995	10.332	O	HETATM 870	C	0	5.709	-12.776	-3.641	C
HETATM 783	N	0	-6.465	-11.665	9.383	N	HETATM 871	O	0	6.817	-12.743	-4.175	O
HETATM 784	N	0	-1.309	-9.134	9.721	N	HETATM 872	C	0	4.100	-12.407	-5.565	C

HETATM 873	C	0	2.924	-13.009	-6.332	C	HETATM 961	C	0	20.882	-5.153	-4.015	C
HETATM 874	C	0	2.354	-12.065	-7.367	C	HETATM 962	C	0	20.950	-6.687	-4.079	C
HETATM 875	N	0	3.310	-11.935	-8.472	N	HETATM 963	N	0	20.441	-7.307	-2.844	N
HETATM 876	C	0	3.046	-11.253	-9.577	C	HETATM 964	C	0	19.825	-8.493	-2.770	C
HETATM 877	N	0	1.865	-10.666	-9.694	N	HETATM 965	N	0	19.611	-9.218	-3.862	N
HETATM 878	N	0	3.944	-11.182	-10.567	N	HETATM 966	N	0	19.397	-8.948	-1.590	N
HETATM 879	N	0	5.509	-12.355	-2.390	N	HETATM 967	N	0	20.683	-1.480	-3.523	N
HETATM 880	C	0	6.573	-11.715	-1.620	C	HETATM 968	C	0	21.280	-0.373	-4.241	C
HETATM 881	C	0	6.971	-12.484	-0.373	C	HETATM 969	C	0	20.665	0.993	-3.989	C
HETATM 882	O	0	8.179	-12.634	-0.079	O	HETATM 970	O	0	21.198	1.999	-4.442	O
HETATM 883	C	0	6.147	-10.295	-1.175	C	HETATM 971	N	0	19.549	1.043	-3.278	N
HETATM 884	S	0	5.799	-9.204	-2.577	S	HETATM 972	C	0	18.876	2.326	-3.096	C
HETATM 885	N	0	5.964	-12.910	0.397	N	HETATM 973	C	0	19.555	3.215	-2.032	C
HETATM 886	C	0	6.181	-13.680	1.619	C	HETATM 974	O	0	19.838	2.761	-0.930	O
HETATM 887	C	0	7.197	-14.806	1.413	C	HETATM 975	C	0	17.418	2.106	-2.705	C
HETATM 888	O	0	7.050	-15.611	0.495	O	HETATM 976	S	0	16.513	1.017	-3.840	S
HETATM 889	C	0	4.843	-14.262	2.080	C	HETATM 977	N	0	19.760	4.484	-2.372	N
HETATM 890	C	0	4.866	-14.936	3.446	C	HETATM 978	C	0	20.145	5.461	-1.367	C
HETATM 891	C	0	3.420	-15.292	3.804	C	HETATM 979	C	0	18.851	5.848	-0.679	C
HETATM 892	C	0	3.310	-15.930	5.192	C	HETATM 980	O	0	17.963	6.458	-1.305	O
HETATM 893	N	0	1.895	-16.286	5.467	N	HETATM 981	C	0	20.843	6.670	-2.000	C
HETATM 894	N	0	8.226	-14.839	2.262	N	HETATM 982	C	0	21.100	7.831	-1.025	C
HETATM 895	C	0	9.233	-15.908	2.236	C	HETATM 983	C	0	22.300	8.711	-1.400	C
HETATM 896	C	0	10.362	-15.684	1.234	C	HETATM 984	N	0	22.694	8.704	-2.816	N
HETATM 897	O	0	11.398	-16.354	1.296	O	HETATM 985	C	0	21.930	9.094	-3.842	C
HETATM 898	N	0	10.189	-14.737	0.318	N	HETATM 986	N	0	20.683	9.500	-3.645	N
HETATM 899	C	0	11.205	-14.472	-0.701	C	HETATM 987	N	0	22.413	9.053	-5.084	N
HETATM 900	C	0	12.308	-13.533	-0.220	C	HETATM 988	N	0	18.747	5.485	0.596	N
HETATM 901	O	0	12.242	-12.966	0.881	O	HETATM 989	C	0	17.479	5.541	1.351	C
HETATM 902	C	0	10.550	-13.914	-2.013	C	HETATM 990	C	0	17.482	6.614	2.444	C
HETATM 903	O	0	10.186	-12.533	-1.827	O	HETATM 991	O	0	16.659	7.536	2.404	O
HETATM 904	C	0	9.365	-14.737	-2.385	C	HETATM 992	C	0	17.170	4.194	1.995	C
HETATM 905	N	0	13.325	-13.347	-1.066	N	HETATM 993	C	0	16.879	3.011	1.083	C
HETATM 906	C	0	14.393	-12.402	-0.744	C	HETATM 994	C	0	16.902	1.728	1.903	C
HETATM 907	C	0	13.903	-10.982	-1.030	C	HETATM 995	C	0	15.538	3.207	0.389	C
HETATM 908	O	0	14.246	-10.387	-2.049	O	HETATM 996	O	0	18.279	6.563	3.386	O
HETATM 909	C	0	15.658	-12.741	-1.549	C	HETATM 997	Re	0	6.933	12.924	1.660	Re
HETATM 910	C	0	16.835	-11.788	-1.271	C	HETATM 998	C	0	6.117	12.539	-0.019	C
HETATM 911	O	0	16.807	-10.997	-0.302	O	HETATM 999	O	0	5.603	12.274	-1.059	O
HETATM 912	O	0	17.878	-11.858	-2.109	O	HETATM 1000	C	0	7.860	14.429	0.903	C
HETATM 913	N	0	13.077	-10.454	-0.119	N	HETATM 1001	O	0	8.400	15.383	0.450	O
HETATM 914	C	0	12.486	-9.107	-0.299	C	HETATM 1002	C	0	8.421	11.821	1.146	C
HETATM 915	C	0	13.508	-7.958	-0.212	C	HETATM 1003	O	0	9.377	11.216	0.799	O
HETATM 916	O	0	13.273	-6.886	-0.744	O	HETATM 1004	H	0	2.437	8.933	-8.329	H
HETATM 917	C	0	11.280	-8.848	0.650	C	HETATM 1005	H	0	2.457	10.490	-9.229	H
HETATM 918	C	0	10.158	-9.865	0.372	C	HETATM 1006	H	0	4.765	8.468	-8.900	H
HETATM 919	C	0	11.721	-8.912	2.106	C	HETATM 1007	H	0	4.816	9.824	-10.091	H
HETATM 920	N	0	14.657	-8.202	0.420	N	HETATM 1008	H	0	4.335	10.178	-7.063	H
HETATM 921	C	0	15.713	-7.207	0.505	C	HETATM 1009	H	0	4.532	11.483	-8.300	H
HETATM 922	C	0	16.181	-6.810	-0.904	C	HETATM 1010	H	0	6.688	9.412	-7.543	H
HETATM 923	O	0	16.713	-5.713	-1.089	O	HETATM 1011	H	0	6.844	10.717	-8.779	H
HETATM 924	C	0	16.861	-7.862	1.267	C	HETATM 1012	H	0	6.416	11.006	-5.862	H
HETATM 925	C	0	17.859	-6.993	1.950	C	HETATM 1013	H	0	7.760	11.452	-6.758	H
HETATM 926	C	0	18.843	-7.900	2.675	C	HETATM 1014	H	0	2.748	9.327	-11.374	H
HETATM 927	O	0	18.669	-8.200	3.863	O	HETATM 1015	H	0	0.604	8.327	-11.472	H
HETATM 928	N	0	19.832	-8.427	1.931	N	HETATM 1016	H	0	0.572	9.753	-10.599	H
HETATM 929	N	0	16.032	-7.720	-1.878	N	HETATM 1017	H	0	5.185	5.744	-13.476	H
HETATM 930	C	0	16.374	-7.411	-3.283	C	HETATM 1018	H	0	5.717	3.557	-11.790	H
HETATM 931	C	0	15.691	-6.131	-3.812	C	HETATM 1019	H	0	4.782	2.950	-13.136	H
HETATM 932	O	0	16.258	-5.362	-4.612	O	HETATM 1020	H	0	6.274	3.811	-13.427	H
HETATM 933	C	0	16.086	-8.611	-4.212	C	HETATM 1021	H	0	2.483	5.184	-12.820	H
HETATM 934	N	0	14.455	-5.904	-3.343	N	HETATM 1022	H	0	3.099	3.786	-13.667	H
HETATM 935	C	0	13.663	-4.757	-3.753	C	HETATM 1023	H	0	3.174	5.363	-14.414	H
HETATM 936	C	0	14.253	-3.420	-3.330	C	HETATM 1024	H	0	3.959	5.047	-10.849	H
HETATM 937	O	0	13.941	-2.388	-3.916	O	HETATM 1025	H	0	6.475	4.291	-7.365	H
HETATM 938	C	0	12.221	-4.884	-3.224	C	HETATM 1026	H	0	8.202	4.885	-7.049	H
HETATM 939	C	0	11.534	-5.984	-3.965	C	HETATM 1027	H	0	8.601	6.774	-5.838	H
HETATM 940	C	0	11.260	-7.222	-3.516	C	HETATM 1028	H	0	4.609	5.869	-7.087	H
HETATM 941	C	0	11.092	-5.927	-5.324	C	HETATM 1029	H	0	7.756	8.586	-4.381	H
HETATM 942	N	0	10.658	-7.972	-4.508	N	HETATM 1030	H	0	3.759	7.705	-5.689	H
HETATM 943	C	0	10.535	-7.202	-5.632	C	HETATM 1031	H	0	5.309	9.078	-4.335	H
HETATM 944	C	0	11.108	-4.928	-6.310	C	HETATM 1032	H	0	7.673	6.473	-8.968	H
HETATM 945	C	0	10.008	-7.506	-6.873	C	HETATM 1033	H	0	10.413	3.286	-10.276	H
HETATM 946	C	0	10.586	-5.225	-7.567	C	HETATM 1034	H	0	11.609	4.565	-9.670	H
HETATM 947	C	0	10.046	-6.525	-7.836	C	HETATM 1035	H	0	11.675	-0.557	-8.238	H
HETATM 948	N	0	15.106	-3.444	-2.303	N	HETATM 1036	H	0	13.292	0.332	-8.062	H
HETATM 949	C	0	15.740	-2.207	-1.881	C	HETATM 1037	H	0	11.897	-1.389	-6.163	H
HETATM 950	C	0	17.253	-2.194	-2.184	C	HETATM 1038	H	0	13.499	-0.479	-5.962	H
HETATM 951	O	0	17.953	-1.261	-1.778	O	HETATM 1039	H	0	13.776	-2.864	-6.441	H
HETATM 952	C	0	15.439	-1.851	-0.383	C	HETATM 1040	H	0	12.954	-2.504	-8.062	H
HETATM 953	C	0	16.087	-2.843	0.594	C	HETATM 1041	H	0	14.887	-1.620	-8.794	H
HETATM 954	C	0	13.907	-1.631	-0.162	C	HETATM 1042	H	0	10.691	0.948	-6.729	H
HETATM 955	C	0	16.062	-2.376	2.089	C	HETATM 1043	H	0	10.932	6.227	-6.954	H
HETATM 956	N	0	17.720	-3.208	-2.907	N	HETATM 1044	H	0	12.483	7.229	-7.106	H
HETATM 957	C	0	19.161	-3.352	-3.202	C	HETATM 1045	H	0	10.041	7.894	-5.638	H
HETATM 958	C	0	19.642	-2.151	-4.014	C	HETATM 1046	H	0	11.556	8.910	-5.968	H
HETATM 959	O	0	19.062	-1.794	-5.018	O	HETATM 1047	H	0	12.771	7.043	-4.757	H
HETATM 960	C	0	19.403	-4.678	-3.950	C	HETATM 1048	H	0	7.856	3.904	-5.128	H

HETATM 1049	H	0	8.891	2.554	-4.392	H	HETATM 1137	H	0	10.633	1.738	2.038	H
HETATM 1050	H	0	7.436	2.603	-2.476	H	HETATM 1138	H	0	10.082	-1.439	3.891	H
HETATM 1051	H	0	5.362	3.819	-2.461	H	HETATM 1139	H	0	12.304	-5.401	1.204	H
HETATM 1052	H	0	6.737	4.896	-2.507	H	HETATM 1140	H	0	11.681	-3.997	0.167	H
HETATM 1053	H	0	5.802	4.612	-3.955	H	HETATM 1141	H	0	6.747	-6.861	3.359	H
HETATM 1054	H	0	5.521	1.520	-3.592	H	HETATM 1142	H	0	8.172	-5.943	4.108	H
HETATM 1055	H	0	6.017	2.214	-5.117	H	HETATM 1143	H	0	8.312	-7.081	1.380	H
HETATM 1056	H	0	7.029	1.029	-4.327	H	HETATM 1144	H	0	5.904	-1.001	1.844	H
HETATM 1057	H	0	8.650	5.378	-3.431	H	HETATM 1145	H	0	7.626	-1.550	2.254	H
HETATM 1058	H	0	13.140	1.594	-0.435	H	HETATM 1146	H	0	8.040	-2.183	4.748	H
HETATM 1059	H	0	12.439	1.073	-1.948	H	HETATM 1147	H	0	3.454	-1.772	2.492	H
HETATM 1060	H	0	13.423	2.515	-1.892	H	HETATM 1148	H	0	1.425	-2.097	3.874	H
HETATM 1061	H	0	10.756	2.140	-0.552	H	HETATM 1149	H	0	3.781	-2.676	7.397	H
HETATM 1062	H	0	13.734	8.032	-0.426	H	HETATM 1150	H	0	1.595	-2.585	6.270	H
HETATM 1063	H	0	12.872	7.388	-1.803	H	HETATM 1151	H	0	5.374	-3.359	1.477	H
HETATM 1064	H	0	14.373	6.655	-1.291	H	HETATM 1152	H	0	7.174	-4.076	2.781	H
HETATM 1065	H	0	13.338	5.948	0.784	H	HETATM 1153	H	0	10.290	-2.788	-1.790	H
HETATM 1066	H	0	7.403	8.381	-0.677	H	HETATM 1154	H	0	9.140	-2.016	-4.242	H
HETATM 1067	H	0	8.072	6.967	-1.457	H	HETATM 1155	H	0	10.365	-0.835	-3.841	H
HETATM 1068	H	0	8.767	8.541	-1.757	H	HETATM 1156	H	0	10.781	-2.530	-3.930	H
HETATM 1069	H	0	9.478	8.688	0.533	H	HETATM 1157	H	0	9.117	-0.353	-0.893	H
HETATM 1070	H	0	7.812	2.658	2.545	H	HETATM 1158	H	0	10.771	-0.877	-0.684	H
HETATM 1071	H	0	8.870	3.096	1.088	H	HETATM 1159	H	0	10.322	0.058	-2.089	H
HETATM 1072	H	0	5.937	3.032	1.346	H	HETATM 1160	H	0	7.589	-1.522	-2.223	H
HETATM 1073	H	0	6.938	3.642	-0.090	H	HETATM 1161	H	0	2.137	-5.346	-0.855	H
HETATM 1074	H	0	4.606	2.031	-0.267	H	HETATM 1162	H	0	3.490	-6.162	-0.109	H
HETATM 1075	H	0	4.703	0.311	0.024	H	HETATM 1163	H	0	3.555	-4.438	-0.389	H
HETATM 1076	H	0	5.138	0.958	-1.539	H	HETATM 1164	H	0	3.473	-6.578	-2.483	H
HETATM 1077	H	0	6.990	5.016	2.278	H	HETATM 1165	H	0	4.866	-1.195	-2.888	H
HETATM 1078	H	0	12.480	4.075	3.954	H	HETATM 1166	H	0	3.490	-0.305	-3.493	H
HETATM 1079	H	0	12.572	5.905	3.679	H	HETATM 1167	H	0	4.793	-0.739	-4.573	H
HETATM 1080	H	0	12.846	4.460	6.237	H	HETATM 1168	H	0	2.462	-2.228	-3.938	H
HETATM 1081	H	0	13.121	6.250	5.843	H	HETATM 1169	H	0	6.475	-5.331	-6.355	H
HETATM 1082	H	0	14.686	3.907	4.945	H	HETATM 1170	H	0	7.334	-3.817	-6.991	H
HETATM 1083	H	0	14.974	5.705	4.604	H	HETATM 1171	H	0	6.050	-5.811	-8.666	H
HETATM 1084	H	0	14.995	4.374	7.245	H	HETATM 1172	H	0	7.828	-5.853	-8.143	H
HETATM 1085	H	0	15.516	6.086	6.765	H	HETATM 1173	H	0	6.443	-3.705	-9.643	H
HETATM 1086	H	0	17.359	4.646	7.200	H	HETATM 1174	H	0	8.242	-3.903	-9.246	H
HETATM 1087	H	0	17.296	5.109	5.635	H	HETATM 1175	H	0	6.558	-5.576	-11.022	H
HETATM 1088	H	0	10.559	4.428	5.298	H	HETATM 1176	H	0	8.369	-5.716	-10.658	H
HETATM 1089	H	0	6.667	5.984	9.027	H	HETATM 1177	H	0	7.091	-4.217	-12.592	H
HETATM 1090	H	0	8.442	5.546	8.727	H	HETATM 1178	H	0	8.687	-4.341	-12.272	H
HETATM 1091	H	0	6.501	0.888	5.189	H	HETATM 1179	H	0	5.305	-2.962	-7.762	H
HETATM 1092	H	0	6.817	2.673	4.806	H	HETATM 1180	H	0	3.180	-7.945	-5.763	H
HETATM 1093	H	0	4.629	3.173	5.258	H	HETATM 1181	H	0	2.357	-8.754	-7.213	H
HETATM 1094	H	0	3.488	1.821	3.492	H	HETATM 1182	H	0	5.161	-8.969	-5.322	H
HETATM 1095	H	0	4.780	0.648	3.582	H	HETATM 1183	H	0	4.028	-8.295	-9.377	H
HETATM 1096	H	0	5.106	2.265	3.006	H	HETATM 1184	H	0	7.316	-9.872	-6.069	H
HETATM 1097	H	0	2.875	1.596	5.917	H	HETATM 1185	H	0	6.267	-9.096	-10.135	H
HETATM 1098	H	0	4.100	1.768	7.151	H	HETATM 1186	H	0	7.902	-9.876	-8.441	H
HETATM 1099	H	0	4.079	0.348	6.133	H	HETATM 1187	H	0	2.925	-6.779	-8.472	H
HETATM 1100	H	0	6.054	1.930	7.548	H	HETATM 1188	H	0	-1.465	-3.664	-4.988	H
HETATM 1101	H	0	11.681	2.371	7.941	H	HETATM 1189	H	0	0.368	-3.584	-4.728	H
HETATM 1102	H	0	11.552	2.154	6.105	H	HETATM 1190	H	0	-0.857	-4.508	-2.870	H
HETATM 1103	H	0	10.387	0.106	6.535	H	HETATM 1191	H	0	0.243	-5.721	-3.737	H
HETATM 1104	H	0	10.684	-2.191	11.700	H	HETATM 1192	H	0	-0.948	-5.682	-6.361	H
HETATM 1105	H	0	11.686	-1.198	10.498	H	HETATM 1193	H	0	-0.771	-0.732	-6.902	H
HETATM 1106	H	0	9.661	-2.886	9.296	H	HETATM 1194	H	0	-0.357	0.305	-8.381	H
HETATM 1107	H	0	5.069	-0.641	8.945	H	HETATM 1195	H	0	1.037	0.614	-6.554	H
HETATM 1108	H	0	5.927	0.891	9.537	H	HETATM 1196	H	0	-0.856	-2.035	-9.071	H
HETATM 1109	H	0	5.020	2.161	11.352	H	HETATM 1197	H	0	2.475	-3.010	-12.005	H
HETATM 1110	H	0	3.023	-1.324	9.943	H	HETATM 1198	H	0	2.746	-1.200	-12.295	H
HETATM 1111	H	0	3.009	2.788	12.657	H	HETATM 1199	H	0	4.114	-2.646	-10.161	H
HETATM 1112	H	0	1.009	-0.688	11.228	H	HETATM 1200	H	0	6.016	2.273	-8.303	H
HETATM 1113	H	0	0.141	0.715	12.794	H	HETATM 1201	H	0	5.781	1.244	-9.827	H
HETATM 1114	H	0	6.470	-0.369	11.547	H	HETATM 1202	H	0	5.660	0.107	-6.317	H
HETATM 1115	H	0	7.667	-6.565	12.356	H	HETATM 1203	H	0	7.902	0.345	-9.932	H
HETATM 1116	H	0	8.975	-5.254	12.277	H	HETATM 1204	H	0	7.280	-1.516	-5.412	H
HETATM 1117	H	0	6.044	-4.598	7.765	H	HETATM 1205	H	0	9.572	-1.160	-9.015	H
HETATM 1118	H	0	6.728	-5.568	6.342	H	HETATM 1206	H	0	9.222	-2.210	-6.790	H
HETATM 1119	H	0	6.369	-7.935	6.208	H	HETATM 1207	H	0	4.067	1.163	-7.357	H
HETATM 1120	H	0	4.650	-5.617	9.384	H	HETATM 1208	H	0	-0.000	1.870	-10.935	H
HETATM 1121	H	0	4.822	-9.806	6.733	H	HETATM 1209	H	0	1.496	2.320	-11.932	H
HETATM 1122	H	0	3.110	-7.488	9.920	H	HETATM 1210	H	0	1.947	4.019	-10.301	H
HETATM 1123	H	0	2.565	-9.711	9.427	H	HETATM 1211	H	0	-0.787	7.076	-6.224	H
HETATM 1124	H	0	8.211	-6.617	8.029	H	HETATM 1212	H	0	1.524	7.816	-6.114	H
HETATM 1125	H	0	12.562	-5.881	7.025	H	HETATM 1213	H	0	1.380	6.131	-5.676	H
HETATM 1126	H	0	13.019	-4.717	5.657	H	HETATM 1214	H	0	1.983	6.575	-7.254	H
HETATM 1127	H	0	11.021	-6.286	4.964	H	HETATM 1215	H	0	-0.026	8.643	-7.791	H
HETATM 1128	H	0	11.376	-3.772	7.192	H	HETATM 1216	H	0	-0.387	4.689	-6.758	H
HETATM 1129	H	0	12.841	-1.068	4.097	H	HETATM 1217	H	0	-4.499	6.582	-11.473	H
HETATM 1130	H	0	12.361	-1.126	2.307	H	HETATM 1218	H	0	-2.770	6.027	-11.844	H
HETATM 1131	H	0	11.998	0.939	4.341	H	HETATM 1219	H	0	-3.519	8.327	-10.122	H
HETATM 1132	H	0	12.996	2.329	2.532	H	HETATM 1220	H	0	-1.892	7.872	-10.883	H
HETATM 1133	H	0	14.045	1.013	3.001	H	HETATM 1221	H	0	-4.013	6.141	-9.127	H
HETATM 1134	H	0	13.113	0.905	1.527	H	HETATM 1222	H	0	-3.562	-0.237	-9.915	H
HETATM 1135	H	0	9.917	0.281	2.682	H	HETATM 1223	H	0	-3.003	0.813	-8.636	H
HETATM 1136	H	0	10.116	1.682	3.706	H	HETATM 1224	H	0	-2.213	0.838	-10.194	H

HETATM 1225	H	0	-4.270	1.745	-11.225	H	HETATM 1313	H	0	-4.052	1.161	2.579	H
HETATM 1226	H	0	-9.769	1.446	-9.424	H	HETATM 1314	H	0	-3.367	1.733	1.076	H
HETATM 1227	H	0	-9.369	3.883	-9.534	H	HETATM 1315	H	0	-6.436	-1.735	0.002	H
HETATM 1228	H	0	-8.450	3.134	-8.250	H	HETATM 1316	H	0	-10.501	-3.795	0.742	H
HETATM 1229	H	0	-7.661	3.582	-9.744	H	HETATM 1317	H	0	-9.387	-4.289	-0.654	H
HETATM 1230	H	0	-9.703	2.674	-11.473	H	HETATM 1318	H	0	-10.251	-2.224	-1.785	H
HETATM 1231	H	0	-7.641	0.730	-8.539	H	HETATM 1319	H	0	-15.000	0.890	-1.261	H
HETATM 1232	H	0	-7.669	-3.662	-8.773	H	HETATM 1320	H	0	-13.465	0.905	-2.299	H
HETATM 1233	H	0	-8.520	-4.743	-10.015	H	HETATM 1321	H	0	-14.386	-1.544	-2.093	H
HETATM 1234	H	0	-9.323	-2.632	-11.003	H	HETATM 1322	H	0	-12.951	0.600	0.087	H
HETATM 1235	H	0	-13.796	-4.717	-11.139	H	HETATM 1323	H	0	-13.495	-4.718	1.490	H
HETATM 1236	H	0	-13.724	-2.870	-11.002	H	HETATM 1324	H	0	-14.573	-4.919	-0.005	H
HETATM 1237	H	0	-15.283	-4.447	-9.093	H	HETATM 1325	H	0	-15.798	-5.392	2.544	H
HETATM 1238	H	0	-15.966	-4.029	-10.764	H	HETATM 1326	H	0	-14.528	-6.617	1.977	H
HETATM 1239	H	0	-14.877	-2.193	-8.749	H	HETATM 1327	H	0	-16.332	-7.504	1.095	H
HETATM 1240	H	0	-15.719	-1.834	-10.360	H	HETATM 1328	H	0	-15.967	-6.200	-0.170	H
HETATM 1241	H	0	-13.002	-3.328	-8.654	H	HETATM 1329	H	0	-17.792	-5.627	1.996	H
HETATM 1242	H	0	-13.961	-6.302	-5.423	H	HETATM 1330	H	0	-16.016	-3.245	0.918	H
HETATM 1243	H	0	-13.161	-7.973	-5.438	H	HETATM 1331	H	0	-12.220	-2.882	6.090	H
HETATM 1244	H	0	-12.538	-7.610	-7.710	H	HETATM 1332	H	0	-11.656	-3.262	4.366	H
HETATM 1245	H	0	-16.594	-11.757	-8.361	H	HETATM 1333	H	0	-12.096	-5.631	3.593	H
HETATM 1246	H	0	-14.518	-12.591	-9.357	H	HETATM 1334	H	0	-14.593	-3.219	7.337	H
HETATM 1247	H	0	-15.094	-11.180	-10.210	H	HETATM 1335	H	0	-16.327	-4.454	8.619	H
HETATM 1248	H	0	-13.765	-11.038	-9.086	H	HETATM 1336	H	0	-15.632	-7.982	6.289	H
HETATM 1249	H	0	-14.970	-11.003	-6.340	H	HETATM 1337	H	0	-16.839	-6.801	8.077	H
HETATM 1250	H	0	-16.147	-9.378	-9.064	H	HETATM 1338	H	0	-14.399	-2.169	4.998	H
HETATM 1251	H	0	-18.370	-8.819	-2.983	H	HETATM 1339	H	0	-8.966	0.944	4.308	H
HETATM 1252	H	0	-17.028	-9.932	-3.612	H	HETATM 1340	H	0	-9.665	0.117	2.804	H
HETATM 1253	H	0	-18.762	-9.343	-5.276	H	HETATM 1341	H	0	-9.344	-2.361	2.708	H
HETATM 1254	H	0	-19.358	-5.052	-5.982	H	HETATM 1342	H	0	-9.187	0.430	6.944	H
HETATM 1255	H	0	-18.188	-4.964	-7.417	H	HETATM 1343	H	0	-8.676	-0.710	9.098	H
HETATM 1256	H	0	-15.936	-4.409	-2.228	H	HETATM 1344	H	0	-8.361	-4.509	7.142	H
HETATM 1257	H	0	-14.471	-3.301	-2.476	H	HETATM 1345	H	0	-8.250	-3.148	9.162	H
HETATM 1258	H	0	-13.856	-5.461	-2.326	H	HETATM 1346	H	0	-11.184	0.788	5.327	H
HETATM 1259	H	0	-16.303	-2.639	-3.812	H	HETATM 1347	H	0	-16.409	5.851	2.619	H
HETATM 1260	H	0	-13.212	0.299	-5.797	H	HETATM 1348	H	0	-15.681	7.161	1.527	H
HETATM 1261	H	0	-12.339	0.835	-8.028	H	HETATM 1349	H	0	-15.899	4.234	0.981	H
HETATM 1262	H	0	-11.108	0.126	-7.010	H	HETATM 1350	H	0	-14.397	4.015	-3.321	H
HETATM 1263	H	0	-11.881	-0.838	-8.246	H	HETATM 1351	H	0	-15.444	4.569	-4.746	H
HETATM 1264	H	0	-14.650	-1.607	-7.042	H	HETATM 1352	H	0	-15.613	6.090	-2.942	H
HETATM 1265	H	0	-12.546	-2.545	-6.451	H	HETATM 1353	H	0	-20.379	5.555	-1.643	H
HETATM 1266	H	0	-7.106	-2.698	-4.753	H	HETATM 1354	H	0	-19.870	6.440	-3.190	H
HETATM 1267	H	0	-8.210	-3.254	-6.134	H	HETATM 1355	H	0	-20.761	1.789	-6.619	H
HETATM 1268	H	0	-9.124	-1.635	-3.820	H	HETATM 1356	H	0	-20.425	3.587	-6.318	H
HETATM 1269	H	0	-8.023	2.535	-3.239	H	HETATM 1357	H	0	-18.482	1.419	-5.899	H
HETATM 1270	H	0	-7.568	3.686	-4.619	H	HETATM 1358	H	0	-18.251	3.242	-6.142	H
HETATM 1271	H	0	-9.139	4.288	-6.255	H	HETATM 1359	H	0	-19.316	1.410	-8.177	H
HETATM 1272	H	0	-10.119	1.333	-3.317	H	HETATM 1360	H	0	-18.521	3.077	-8.324	H
HETATM 1273	H	0	-11.512	4.336	-6.981	H	HETATM 1361	H	0	-21.659	2.495	-4.471	H
HETATM 1274	H	0	-12.481	1.398	-4.023	H	HETATM 1362	H	0	-18.099	-0.208	-0.951	H
HETATM 1275	H	0	-13.969	2.370	-5.338	H	HETATM 1363	H	0	-18.884	-2.776	-1.745	H
HETATM 1276	H	0	-7.299	1.666	-6.035	H	HETATM 1364	H	0	-17.709	-2.311	-0.539	H
HETATM 1277	H	0	-3.755	3.305	-4.297	H	HETATM 1365	H	0	-17.211	-2.551	-2.197	H
HETATM 1278	H	0	-3.441	3.552	-6.107	H	HETATM 1366	H	0	-17.933	0.164	-3.576	H
HETATM 1279	H	0	1.934	1.813	-3.968	H	HETATM 1367	H	0	-19.943	-1.243	-3.117	H
HETATM 1280	H	0	1.153	3.222	-6.205	H	HETATM 1368	H	0	-24.880	-2.235	-0.685	H
HETATM 1281	H	0	1.685	4.373	-5.004	H	HETATM 1369	H	0	-23.581	-3.440	-1.228	H
HETATM 1282	H	0	2.735	3.062	-5.482	H	HETATM 1370	H	0	-24.375	-0.816	-2.509	H
HETATM 1283	H	0	0.350	2.361	-2.259	H	HETATM 1371	H	0	-24.317	-2.505	-3.270	H
HETATM 1284	H	0	0.378	4.046	-3.029	H	HETATM 1372	H	0	-22.043	-2.560	-3.175	H
HETATM 1285	H	0	1.928	3.876	-1.117	H	HETATM 1373	H	0	-22.277	-0.735	-3.397	H
HETATM 1286	H	0	2.729	2.540	-1.909	H	HETATM 1374	H	0	-23.217	-0.689	-0.002	H
HETATM 1287	H	0	2.755	4.129	-2.635	H	HETATM 1375	H	0	-23.194	-2.233	3.953	H
HETATM 1288	H	0	0.030	1.473	-5.797	H	HETATM 1376	H	0	-22.749	-3.719	2.939	H
HETATM 1289	H	0	-1.061	-1.612	-0.225	H	HETATM 1377	H	0	-19.326	0.302	1.869	H
HETATM 1290	H	0	-1.205	0.227	-0.407	H	HETATM 1378	H	0	-18.654	-1.236	1.082	H
HETATM 1291	H	0	1.134	0.135	-1.211	H	HETATM 1379	H	0	-17.033	-0.273	2.885	H
HETATM 1292	H	0	0.107	0.163	1.437	H	HETATM 1380	H	0	-18.566	-2.291	3.188	H
HETATM 1293	H	0	1.624	-0.704	1.478	H	HETATM 1381	H	0	-16.209	0.201	7.814	H
HETATM 1294	H	0	1.565	0.924	0.847	H	HETATM 1382	H	0	-15.575	-1.122	6.683	H
HETATM 1295	H	0	0.792	-2.660	-1.035	H	HETATM 1383	H	0	-16.771	-2.125	8.404	H
HETATM 1296	H	0	2.006	-2.210	0.137	H	HETATM 1384	H	0	-17.855	-2.043	6.903	H
HETATM 1297	H	0	2.210	-1.774	-1.543	H	HETATM 1385	H	0	-19.144	-1.591	8.831	H
HETATM 1298	H	0	-0.568	-1.617	-2.642	H	HETATM 1386	H	0	-18.770	-0.003	7.952	H
HETATM 1299	H	0	-5.269	-3.530	-4.573	H	HETATM 1387	H	0	-17.605	0.677	9.768	H
HETATM 1300	H	0	-3.537	-3.514	-3.913	H	HETATM 1388	H	0	-17.811	0.793	6.204	H
HETATM 1301	H	0	-3.569	-3.674	-6.290	H	HETATM 1389	H	0	-15.924	4.702	6.151	H
HETATM 1302	H	0	-3.033	-1.993	-5.724	H	HETATM 1390	H	0	-15.869	4.182	4.373	H
HETATM 1303	H	0	-5.091	-0.385	-7.803	H	HETATM 1391	H	0	-13.992	2.873	4.837	H
HETATM 1304	H	0	-4.431	-0.176	-6.216	H	HETATM 1392	H	0	-10.772	0.925	9.157	H
HETATM 1305	H	0	-5.169	-1.082	-4.358	H	HETATM 1393	H	0	-11.880	0.366	7.781	H
HETATM 1306	H	0	-6.251	1.227	-0.360	H	HETATM 1394	H	0	-11.881	-0.149	10.578	H
HETATM 1307	H	0	-8.041	-0.126	1.322	H	HETATM 1395	H	0	-14.291	-0.190	10.875	H
HETATM 1308	H	0	-6.779	0.552	2.322	H	HETATM 1396	H	0	-13.644	1.425	10.710	H
HETATM 1309	H	0	-7.691	1.584	1.246	H	HETATM 1397	H	0	-14.473	0.674	9.367	H
HETATM 1310	H	0	-4.889	-0.626	1.578	H	HETATM 1398	H	0	-13.190	-2.068	9.866	H
HETATM 1311	H	0	-4.162	-0.019	-0.015	H	HETATM 1399	H	0	-13.220	-1.417	8.245	H
HETATM 1312	H	0	-4.999	2.174	1.516	H	HETATM 1400	H	0	-11.701	-1.886	8.970	H

HETATM 1401	H	0	-12.797	2.630	9.261	H	HETATM 1489	H	0	2.769	6.139	5.983	H
HETATM 1402	H	0	-12.500	9.099	8.400	H	HETATM 1490	H	0	3.689	4.942	5.104	H
HETATM 1403	H	0	-10.847	8.328	8.728	H	HETATM 1491	H	0	2.406	4.687	2.225	H
HETATM 1404	H	0	-11.878	5.912	10.835	H	HETATM 1492	H	0	3.805	5.025	3.217	H
HETATM 1405	H	0	-10.824	7.281	10.713	H	HETATM 1493	H	0	3.025	6.317	2.336	H
HETATM 1406	H	0	-12.951	7.296	6.847	H	HETATM 1494	H	0	0.992	3.794	3.650	H
HETATM 1407	H	0	-9.204	8.718	2.347	H	HETATM 1495	H	0	-2.752	7.130	7.949	H
HETATM 1408	H	0	-9.066	9.789	4.914	H	HETATM 1496	H	0	-2.709	7.454	6.125	H
HETATM 1409	H	0	-7.907	8.485	4.819	H	HETATM 1497	H	0	-0.785	5.731	7.582	H
HETATM 1410	H	0	-7.857	9.784	3.652	H	HETATM 1498	H	0	-0.183	-0.353	4.184	H
HETATM 1411	H	0	-9.263	6.543	4.321	H	HETATM 1499	H	0	-1.111	0.704	3.148	H
HETATM 1412	H	0	-9.996	6.483	2.620	H	HETATM 1500	H	0	-0.013	1.380	4.327	H
HETATM 1413	H	0	-7.853	5.313	2.746	H	HETATM 1501	H	0	-2.533	-0.159	4.922	H
HETATM 1414	H	0	-7.101	6.781	3.322	H	HETATM 1502	H	0	0.068	2.152	10.445	H
HETATM 1415	H	0	-7.792	6.725	1.718	H	HETATM 1503	H	0	-0.751	3.111	9.088	H
HETATM 1416	H	0	-11.042	9.763	3.884	H	HETATM 1504	H	0	2.029	2.138	9.330	H
HETATM 1417	H	0	-13.676	10.427	-0.561	H	HETATM 1505	H	0	1.230	2.859	7.821	H
HETATM 1418	H	0	-12.159	10.063	-1.560	H	HETATM 1506	H	0	1.760	4.199	10.429	H
HETATM 1419	H	0	-12.557	12.021	0.346	H	HETATM 1507	H	0	1.042	4.912	8.876	H
HETATM 1420	H	0	-10.967	11.391	-0.367	H	HETATM 1508	H	0	3.759	3.837	9.305	H
HETATM 1421	H	0	-12.076	11.166	2.253	H	HETATM 1509	H	0	3.036	4.647	7.803	H
HETATM 1422	H	0	-10.425	10.666	1.576	H	HETATM 1510	H	0	2.893	6.342	9.929	H
HETATM 1423	H	0	-13.360	8.284	0.205	H	HETATM 1511	H	0	4.432	5.796	9.901	H
HETATM 1424	H	0	-11.588	9.434	-5.352	H	HETATM 1512	H	0	0.257	0.334	8.786	H
HETATM 1425	H	0	-10.080	10.484	-5.597	H	HETATM 1513	H	0	-6.171	0.687	10.131	H
HETATM 1426	H	0	-10.716	10.532	-3.090	H	HETATM 1514	H	0	-5.334	1.410	8.644	H
HETATM 1427	H	0	-9.527	8.161	-5.226	H	HETATM 1515	H	0	-5.454	2.364	11.395	H
HETATM 1428	H	0	-8.593	9.957	-0.084	H	HETATM 1516	H	0	-4.471	3.049	9.981	H
HETATM 1429	H	0	-6.945	9.521	0.300	H	HETATM 1517	H	0	-7.400	3.033	10.471	H
HETATM 1430	H	0	-7.353	11.187	-0.034	H	HETATM 1518	H	0	-6.594	3.337	8.830	H
HETATM 1431	H	0	-6.987	10.862	-2.222	H	HETATM 1519	H	0	-7.207	5.389	10.016	H
HETATM 1432	H	0	-6.958	5.219	-2.667	H	HETATM 1520	H	0	-5.377	5.129	9.882	H
HETATM 1433	H	0	-5.349	4.577	-2.009	H	HETATM 1521	H	0	-6.309	4.001	12.173	H
HETATM 1434	H	0	-7.426	6.021	-0.411	H	HETATM 1522	H	0	-6.922	5.514	12.150	H
HETATM 1435	H	0	-7.908	3.781	0.484	H	HETATM 1523	H	0	-3.890	0.369	11.030	H
HETATM 1436	H	0	-8.236	3.827	-1.231	H	HETATM 1524	H	0	-3.483	-2.212	5.876	H
HETATM 1437	H	0	-6.772	3.078	-0.642	H	HETATM 1525	H	0	-4.673	-4.745	6.378	H
HETATM 1438	H	0	-6.025	5.262	1.448	H	HETATM 1526	H	0	-5.384	-4.114	4.912	H
HETATM 1439	H	0	-4.916	4.512	0.326	H	HETATM 1527	H	0	-3.651	-4.295	5.035	H
HETATM 1440	H	0	-5.091	6.250	0.351	H	HETATM 1528	H	0	-6.406	-2.411	5.464	H
HETATM 1441	H	0	-4.694	6.817	-1.574	H	HETATM 1529	H	0	-5.591	-0.882	6.122	H
HETATM 1442	H	0	-6.345	8.634	-6.638	H	HETATM 1530	H	0	-6.148	-0.701	3.779	H
HETATM 1443	H	0	-5.356	7.658	-7.864	H	HETATM 1531	H	0	-5.195	-2.129	3.455	H
HETATM 1444	H	0	-7.349	6.674	-5.887	H	HETATM 1532	H	0	-4.426	-0.687	4.075	H
HETATM 1445	H	0	-8.521	6.015	-8.003	H	HETATM 1533	H	0	-5.544	-2.917	7.951	H
HETATM 1446	H	0	-8.265	7.743	-7.949	H	HETATM 1534	H	0	0.041	-3.453	7.176	H
HETATM 1447	H	0	-7.224	6.735	-8.927	H	HETATM 1535	H	0	-0.028	-2.354	9.758	H
HETATM 1448	H	0	-6.980	4.475	-6.804	H	HETATM 1536	H	0	1.608	-2.895	9.467	H
HETATM 1449	H	0	-5.546	5.102	-6.027	H	HETATM 1537	H	0	0.845	-1.782	8.356	H
HETATM 1450	H	0	-5.662	5.092	-7.771	H	HETATM 1538	H	0	0.618	-5.906	8.431	H
HETATM 1451	H	0	-4.106	6.737	-6.022	H	HETATM 1539	H	0	1.956	-4.831	8.755	H
HETATM 1452	H	0	-3.958	11.810	-3.722	H	HETATM 1540	H	0	1.465	-5.143	7.107	H
HETATM 1453	H	0	-2.456	11.116	-3.001	H	HETATM 1541	H	0	-1.460	-5.231	8.252	H
HETATM 1454	H	0	-2.377	13.374	-3.167	H	HETATM 1542	H	0	-2.295	-2.505	14.060	H
HETATM 1455	H	0	-3.055	11.398	-6.012	H	HETATM 1543	H	0	-3.019	-1.808	12.503	H
HETATM 1456	H	0	1.094	12.274	-8.152	H	HETATM 1544	H	0	-1.067	-0.807	13.309	H
HETATM 1457	H	0	2.658	12.274	-7.281	H	HETATM 1545	H	0	-1.305	-4.245	12.701	H
HETATM 1458	H	0	1.980	13.911	-6.031	H	HETATM 1546	H	0	-7.532	-5.368	11.643	H
HETATM 1459	H	0	1.245	10.298	-6.711	H	HETATM 1547	H	0	-6.400	-4.133	10.849	H
HETATM 1460	H	0	-0.005	13.365	-1.881	H	HETATM 1548	H	0	-5.753	-4.993	13.118	H
HETATM 1461	H	0	1.576	14.193	-2.050	H	HETATM 1549	H	0	-5.260	-9.292	13.209	H
HETATM 1462	H	0	2.757	12.082	-2.393	H	HETATM 1550	H	0	-3.624	-8.928	14.000	H
HETATM 1463	H	0	2.253	6.528	-0.631	H	HETATM 1551	H	0	-4.607	-10.360	8.547	H
HETATM 1464	H	0	2.528	8.081	-2.999	H	HETATM 1552	H	0	-3.605	-11.898	8.290	H
HETATM 1465	H	0	2.926	6.394	-2.779	H	HETATM 1553	H	0	-2.786	-11.546	10.574	H
HETATM 1466	H	0	4.137	7.621	-2.495	H	HETATM 1554	H	0	0.092	-7.674	9.641	H
HETATM 1467	H	0	3.436	7.815	1.007	H	HETATM 1555	H	0	0.644	-9.401	9.255	H
HETATM 1468	H	0	4.379	8.570	-0.399	H	HETATM 1556	H	0	2.761	-8.836	5.289	H
HETATM 1469	H	0	5.644	6.892	0.770	H	HETATM 1557	H	0	2.013	-7.943	3.847	H
HETATM 1470	H	0	4.376	5.733	0.448	H	HETATM 1558	H	0	3.102	-6.947	6.387	H
HETATM 1471	H	0	5.265	6.446	-0.877	H	HETATM 1559	H	0	1.999	-6.000	5.238	H
HETATM 1472	H	0	0.710	8.260	-1.386	H	HETATM 1560	H	0	2.373	-5.791	2.958	H
HETATM 1473	H	0	-0.414	11.785	2.617	H	HETATM 1561	H	0	3.656	-4.629	2.720	H
HETATM 1474	H	0	-0.961	11.100	4.867	H	HETATM 1562	H	0	3.805	-6.242	2.064	H
HETATM 1475	H	0	0.160	12.483	5.019	H	HETATM 1563	H	0	0.181	-7.396	5.408	H
HETATM 1476	H	0	0.779	10.809	5.296	H	HETATM 1564	H	0	-2.006	-12.130	6.456	H
HETATM 1477	H	0	1.425	12.954	3.015	H	HETATM 1565	H	0	-2.328	-13.204	4.981	H
HETATM 1478	H	0	1.361	9.393	3.278	H	HETATM 1566	H	0	-0.839	-11.730	3.762	H
HETATM 1479	H	0	-5.110	8.593	1.881	H	HETATM 1567	H	0	-5.019	-6.852	4.465	H
HETATM 1480	H	0	-4.330	10.156	1.837	H	HETATM 1568	H	0	-4.423	-7.672	5.889	H
HETATM 1481	H	0	-3.920	8.941	0.650	H	HETATM 1569	H	0	-3.305	-6.877	4.806	H
HETATM 1482	H	0	-3.359	8.791	3.613	H	HETATM 1570	H	0	-4.976	-9.294	4.177	H
HETATM 1483	H	0	-1.190	3.757	-0.030	H	HETATM 1571	H	0	-0.472	-7.554	1.122	H
HETATM 1484	H	0	-0.681	5.527	-0.240	H	HETATM 1572	H	0	-1.043	-7.210	-0.608	H
HETATM 1485	H	0	-3.228	5.309	-0.697	H	HETATM 1573	H	0	-2.587	-5.070	-0.937	H
HETATM 1486	H	0	-3.045	4.702	1.299	H	HETATM 1574	H	0	-0.372	-6.618	3.421	H
HETATM 1487	H	0	1.697	6.701	4.092	H	HETATM 1575	H	0	-0.230	-4.981	5.309	H
HETATM 1488	H	0	2.167	4.505	5.843	H	HETATM 1576	H	0	-2.188	-1.985	2.971	H

HETATM 1577	H	0	-1.135	-2.711	5.070	H	HETATM 1665	H	0	15.907	-0.915	-0.157	H
HETATM 1578	H	0	-3.266	-7.745	0.178	H	HETATM 1666	H	0	13.726	-1.389	0.865	H
HETATM 1579	H	0	-5.069	-11.857	-1.319	H	HETATM 1667	H	0	13.378	-2.525	-0.416	H
HETATM 1580	H	0	-5.578	-11.317	-3.629	H	HETATM 1668	H	0	13.569	-0.827	-0.782	H
HETATM 1581	H	0	-4.876	-9.964	-2.774	H	HETATM 1669	H	0	15.484	-3.726	0.555	H
HETATM 1582	H	0	-3.903	-10.894	-3.889	H	HETATM 1670	H	0	17.121	-2.888	0.321	H
HETATM 1583	H	0	-5.005	-13.631	-3.043	H	HETATM 1671	H	0	15.583	-1.422	2.156	H
HETATM 1584	H	0	-3.893	-13.960	-1.736	H	HETATM 1672	H	0	15.521	-3.089	2.676	H
HETATM 1585	H	0	-3.295	-13.345	-3.258	H	HETATM 1673	H	0	17.064	-2.299	2.455	H
HETATM 1586	H	0	-2.860	-12.026	-0.508	H	HETATM 1674	H	0	15.296	-1.432	-2.470	H
HETATM 1587	H	0	-1.023	-8.749	-4.721	H	HETATM 1675	H	0	18.889	-5.424	-3.381	H
HETATM 1588	H	0	0.722	-8.774	-4.629	H	HETATM 1676	H	0	19.120	-4.489	-4.964	H
HETATM 1589	H	0	-0.104	-9.754	-5.816	H	HETATM 1677	H	0	21.336	-4.865	-3.090	H
HETATM 1590	H	0	-0.263	-11.384	-4.430	H	HETATM 1678	H	0	21.279	-4.791	-4.941	H
HETATM 1591	H	0	1.283	-9.273	0.846	H	HETATM 1679	H	0	20.283	-6.985	-4.861	H
HETATM 1592	H	0	2.367	-8.111	-0.109	H	HETATM 1680	H	0	21.988	-6.940	-4.136	H
HETATM 1593	H	0	4.892	-8.086	0.491	H	HETATM 1681	H	0	20.566	-6.800	-1.991	H
HETATM 1594	H	0	1.409	-11.205	2.518	H	HETATM 1682	H	0	19.722	-3.378	-2.291	H
HETATM 1595	H	0	1.976	-12.424	4.596	H	HETATM 1683	H	0	22.283	-0.305	-3.874	H
HETATM 1596	H	0	5.944	-10.830	4.591	H	HETATM 1684	H	0	21.102	-0.578	-5.276	H
HETATM 1597	H	0	4.257	-12.349	5.526	H	HETATM 1685	H	0	20.160	7.050	-2.730	H
HETATM 1598	H	0	3.052	-9.854	-1.477	H	HETATM 1686	H	0	21.809	6.323	-2.300	H
HETATM 1599	H	0	-0.460	-13.318	1.722	H	HETATM 1687	H	0	21.354	7.375	-0.091	H
HETATM 1600	H	0	-0.765	-14.125	0.082	H	HETATM 1688	H	0	20.241	8.465	-1.095	H
HETATM 1601	H	0	0.557	-15.287	2.453	H	HETATM 1689	H	0	21.989	9.714	-1.198	H
HETATM 1602	H	0	0.089	-16.083	0.846	H	HETATM 1690	H	0	23.133	8.293	-0.873	H
HETATM 1603	H	0	-1.590	-15.253	3.143	H	HETATM 1691	H	0	23.615	8.379	-3.031	H
HETATM 1604	H	0	-1.460	-16.885	2.275	H	HETATM 1692	H	0	20.854	5.062	-0.672	H
HETATM 1605	H	0	-3.143	-14.636	1.648	H	HETATM 1693	H	0	16.262	4.352	2.539	H
HETATM 1606	H	0	1.885	-13.541	1.293	H	HETATM 1694	H	0	18.066	3.926	2.516	H
HETATM 1607	H	0	0.132	-14.142	-4.104	H	HETATM 1695	H	0	17.630	2.941	0.324	H
HETATM 1608	H	0	0.680	-15.777	-4.784	H	HETATM 1696	H	0	17.117	1.962	2.925	H
HETATM 1609	H	0	1.606	-16.179	-2.498	H	HETATM 1697	H	0	15.948	1.248	1.840	H
HETATM 1610	H	0	3.747	-11.498	-5.127	H	HETATM 1698	H	0	17.657	1.074	1.520	H
HETATM 1611	H	0	4.929	-12.388	-6.242	H	HETATM 1699	H	0	15.106	4.134	0.703	H
HETATM 1612	H	0	2.148	-13.161	-5.612	H	HETATM 1700	H	0	14.882	2.402	0.648	H
HETATM 1613	H	0	3.320	-13.840	-6.877	H	HETATM 1701	H	0	15.683	3.222	-0.671	H
HETATM 1614	H	0	1.479	-12.533	-7.767	H	HETATM 1702	H	0	16.725	5.794	0.636	H
HETATM 1615	H	0	2.281	-11.103	-6.904	H	HETATM 1703	H	0	14.238	2.443	-4.231	H
HETATM 1616	H	0	4.201	-12.381	-8.387	H	HETATM 1704	H	0	16.123	3.946	-4.563	H
HETATM 1617	H	0	4.857	-14.262	-4.788	H	HETATM 1705	H	0	15.685	3.910	-6.364	H
HETATM 1618	H	0	4.186	-13.424	2.184	H	HETATM 1706	H	0	14.612	9.153	1.708	H
HETATM 1619	H	0	4.612	-15.039	1.381	H	HETATM 1707	H	0	14.992	10.360	-0.293	H
HETATM 1620	H	0	5.197	-14.206	4.154	H	HETATM 1708	H	0	13.385	10.489	0.134	H
HETATM 1621	H	0	5.401	-15.856	3.337	H	HETATM 1709	H	0	16.688	10.258	1.370	H
HETATM 1622	H	0	2.889	-14.365	3.858	H	HETATM 1710	H	0	16.287	10.214	2.988	H
HETATM 1623	H	0	3.115	-16.043	3.105	H	HETATM 1711	H	0	6.358	9.011	6.222	H
HETATM 1624	H	0	3.582	-15.176	5.901	H	HETATM 1712	H	0	4.541	7.866	5.011	H
HETATM 1625	H	0	3.857	-16.849	5.153	H	HETATM 1713	H	0	5.867	7.283	3.855	H
HETATM 1626	H	0	1.826	-16.702	6.374	H	HETATM 1714	H	0	3.567	10.102	4.593	H
HETATM 1627	H	0	1.574	-16.935	4.777	H	HETATM 1715	H	0	7.265	9.724	2.590	H
HETATM 1628	H	0	6.581	-13.025	2.365	H	HETATM 1716	H	0	4.048	12.315	3.381	H
HETATM 1629	H	0	9.695	-15.894	3.201	H	HETATM 1717	H	0	0.202	-1.882	14.575	H
HETATM 1630	H	0	8.717	-16.784	1.902	H	HETATM 1718	H	0	1.863	-1.054	16.027	H
HETATM 1631	H	0	11.256	-13.971	-2.814	H	HETATM 1719	H	0	2.373	-2.562	16.391	H
HETATM 1632	H	0	9.236	-15.520	-1.668	H	HETATM 1720	H	0	-0.456	-3.539	16.676	H
HETATM 1633	H	0	8.491	-14.119	-2.399	H	HETATM 1721	H	0	-1.036	-2.050	16.338	H
HETATM 1634	H	0	9.516	-15.162	-3.355	H	HETATM 1722	H	0	7.920	-5.980	-4.078	H
HETATM 1635	H	0	10.491	-12.235	-0.967	H	HETATM 1723	H	0	7.487	-7.266	-1.421	H
HETATM 1636	H	0	11.670	-15.413	-0.909	H	HETATM 1724	H	0	9.104	-7.138	-2.319	H
HETATM 1637	H	0	15.974	-13.705	-1.207	H	HETATM 1725	H	0	-12.073	4.384	2.988	H
HETATM 1638	H	0	15.400	-12.596	-2.577	H	HETATM 1726	H	0	-11.384	5.049	0.817	H
HETATM 1639	H	0	14.646	-12.472	0.293	H	HETATM 1727	H	0	-10.173	3.910	1.637	H
HETATM 1640	H	0	10.901	-7.865	0.462	H	HETATM 1728	H	0	-8.869	4.570	8.147	H
HETATM 1641	H	0	9.335	-9.677	1.030	H	HETATM 1729	H	0	-9.150	4.123	5.207	H
HETATM 1642	H	0	10.526	-10.857	0.536	H	HETATM 1730	H	0	-7.819	5.162	5.969	H
HETATM 1643	H	0	9.832	-9.769	-0.643	H	HETATM 1731	H	0	-10.201	5.634	-1.161	H
HETATM 1644	H	0	10.879	-8.732	2.741	H	HETATM 1732	H	0	-12.359	5.394	-3.189	H
HETATM 1645	H	0	12.124	-9.881	2.314	H	HETATM 1733	H	0	-10.868	4.305	-3.025	H
HETATM 1646	H	0	12.469	-8.168	2.285	H	HETATM 1734	H	0	-4.870	3.580	6.653	H
HETATM 1647	H	0	12.120	-9.112	-1.305	H	HETATM 1735	H	0	-5.621	4.672	4.678	H
HETATM 1648	H	0	16.387	-8.406	2.058	H	HETATM 1736	H	0	-4.616	3.464	3.695	H
HETATM 1649	H	0	17.421	-8.384	0.520	H	HETATM 1737	H	0	7.414	-11.685	-2.280	H
HETATM 1650	H	0	17.334	-6.436	2.698	H	HETATM 1738	H	0	5.220	-10.413	-0.653	H
HETATM 1651	H	0	18.406	-6.480	1.187	H	HETATM 1739	H	0	6.993	-9.874	-0.674	H
HETATM 1652	H	0	15.371	-6.321	0.997	H	HETATM 1740	H	0	18.939	2.837	-4.034	H
HETATM 1653	H	0	15.694	-9.423	-3.636	H	HETATM 1741	H	0	17.441	1.595	-1.765	H
HETATM 1654	H	0	15.371	-8.323	-4.955	H	HETATM 1742	H	0	16.947	3.064	-2.782	H
HETATM 1655	H	0	16.992	-8.918	-4.690	H	HETATM 1743	H	0	11.808	11.103	4.579	H
HETATM 1656	H	0	17.427	-7.220	-3.289	H	HETATM 1744	H	0	11.217	11.692	2.997	H
HETATM 1657	H	0	12.290	-5.192	-2.202	H	HETATM 1745	H	0	12.760	9.055	3.407	H
HETATM 1658	H	0	11.715	-3.976	-3.477	H	HETATM 1746	H	0	12.124	9.717	1.846	H
HETATM 1659	H	0	11.479	-7.576	-2.531	H	HETATM 1747	C	0	3.374	-4.088	11.938	C
HETATM 1660	H	0	11.512	-3.959	-6.101	H	HETATM 1748	C	0	4.791	-3.783	12.483	C
HETATM 1661	H	0	10.589	-4.480	-8.335	H	HETATM 1749	C	0	10.127	9.979	3.743	C
HETATM 1662	H	0	9.586	-8.468	-7.076	H	HETATM 1750	H	0	9.335	10.733	3.951	H
HETATM 1663	H	0	9.661	-6.737	-8.812	H	HETATM 1751	H	0	9.843	9.504	2.782	H
HETATM 1664	H	0	13.666	-4.765	-4.823	H	HETATM 1752	C	0	2.194	-3.427	12.674	C

HETATM 1753	H	0	4.700	-3.770	13.549	H	HETATM 1841	H	0	-15.718	-9.069	-1.760	H
HETATM 1754	H	0	3.230	-5.148	11.968	H	HETATM 1842	H	0	-5.925	-2.684	-9.361	H
HETATM 1755	H	0	3.341	-3.777	10.914	H	HETATM 1843	H	0	-5.204	-2.738	-10.825	H
HETATM 1756	H	0	2.445	-2.417	12.922	H	HETATM 1844	H	0	-8.870	-1.231	-8.455	H
HETATM 1757	H	0	1.326	-3.440	12.049	H	HETATM 1845	H	0	-6.322	1.095	-11.165	H
HETATM 1758	H	0	2.805	-4.207	14.558	H	HETATM 1846	H	0	-10.303	-7.399	-5.390	H
HETATM 1759	H	0	1.720	-5.239	13.686	H	HETATM 1847	H	0	-11.069	-7.184	-6.816	H
HETATM 1760	H	0	5.341	-1.746	12.791	H	HETATM 1848	H	0	-7.027	-5.327	-3.872	H
HETATM 1761	H	0	-4.159	-8.959	10.534	H	HETATM 1849	H	0	-13.448	-2.750	-0.168	H
HETATM 1762	H	0	-1.759	-8.648	10.470	H	HETATM 1850	H	0	-13.627	-7.564	4.339	H
HETATM 1763	H	0	-8.723	-4.235	4.352	H	HETATM 1851	H	0	-17.371	-6.297	-1.282	H
HETATM 1764	H	0	0.079	-4.413	14.996	H	HETATM 1852	H	0	-18.965	-6.600	-1.470	H
HETATM 1765	H	0	-2.674	3.218	-9.405	H	HETATM 1853	H	0	-19.678	-4.529	1.331	H
HETATM 1766	H	0	-2.039	-9.673	-3.050	H	HETATM 1854	H	0	-20.466	-5.217	-0.042	H
HETATM 1767	H	0	14.177	10.850	3.661	H	HETATM 1855	H	0	-12.974	-2.353	2.462	H
HETATM 1768	C	0	10.166	8.934	4.892	C	HETATM 1856	H	0	-16.257	-0.435	12.181	H
HETATM 1769	H	0	10.935	9.211	5.583	H	HETATM 1857	H	0	-17.762	0.239	12.530	H
HETATM 1770	H	0	8.093	7.616	4.306	H	HETATM 1858	H	0	-17.400	-2.781	11.389	H
HETATM 1771	H	0	10.581	7.445	3.427	H	HETATM 1859	H	0	-18.374	-2.568	10.095	H
HETATM 1772	H	0	8.295	6.560	6.712	H	HETATM 1860	H	0	-16.979	-1.538	4.602	H
HETATM 1773	H	0	20.510	9.580	-2.663	H	HETATM 1861	H	0	-21.025	-0.972	2.465	H
HETATM 1774	H	0	20.050	8.836	-4.042	H	HETATM 1862	H	0	-17.761	8.285	1.331	H
HETATM 1775	H	0	23.140	9.733	-5.182	H	HETATM 1863	H	0	-18.807	7.661	0.244	H
HETATM 1776	H	0	21.679	9.254	-5.733	H	HETATM 1864	H	0	-13.591	5.779	1.849	H
HETATM 1777	H	0	19.567	5.157	1.066	H	HETATM 1865	H	0	-16.391	3.930	-1.096	H
HETATM 1778	H	0	19.649	4.768	-3.324	H	HETATM 1866	H	0	-12.101	-1.148	-1.946	H
HETATM 1779	H	0	19.171	0.212	-2.870	H	HETATM 1867	H	0	-12.121	-0.590	2.945	H
HETATM 1780	H	0	21.061	-1.747	-2.636	H	HETATM 1868	H	0	-15.898	2.117	6.978	H
HETATM 1781	H	0	19.096	-9.897	-1.689	H	HETATM 1869	H	0	-12.625	6.107	5.260	H
HETATM 1782	H	0	20.143	-8.903	-0.925	H	HETATM 1870	H	0	-12.932	5.376	3.833	H
HETATM 1783	H	0	20.199	-10.027	-3.845	H	HETATM 1871	H	0	-12.884	1.587	6.600	H
HETATM 1784	H	0	18.653	-9.503	-3.890	H	HETATM 1872	H	0	-10.751	-6.379	-0.374	H
HETATM 1785	H	0	17.080	-3.890	-3.261	H	HETATM 1873	H	0	-11.960	-6.420	-1.613	H
HETATM 1786	H	0	14.064	-6.548	-2.686	H	HETATM 1874	H	0	-8.398	-2.273	0.483	H
HETATM 1787	H	0	15.305	-4.302	-1.831	H	HETATM 1875	H	0	-10.833	3.214	6.480	H
HETATM 1788	H	0	15.681	-8.628	-1.649	H	HETATM 1876	H	0	-11.826	5.405	7.169	H
HETATM 1789	H	0	10.360	-8.923	-4.419	H	HETATM 1877	H	0	-11.813	7.044	4.618	H
HETATM 1790	H	0	20.463	-8.929	2.522	H	HETATM 1878	H	0	-12.802	6.715	-1.233	H
HETATM 1791	H	0	19.443	-9.051	1.253	H	HETATM 1879	H	0	-3.043	1.713	8.702	H
HETATM 1792	H	0	14.796	-9.095	0.847	H	HETATM 1880	H	0	-12.393	1.543	2.214	H
HETATM 1793	H	0	12.854	-10.980	0.701	H	HETATM 1881	H	0	-11.560	8.067	-3.330	H
HETATM 1794	H	0	8.315	-14.110	2.940	H	HETATM 1882	H	0	-9.344	9.363	-1.942	H
HETATM 1795	H	0	9.349	-14.195	0.326	H	HETATM 1883	H	0	-7.441	7.466	-2.178	H
HETATM 1796	H	0	13.355	-13.858	-1.926	H	HETATM 1884	H	0	-5.883	8.294	-4.232	H
HETATM 1797	H	0	5.027	-12.693	0.125	H	HETATM 1885	H	0	-3.849	9.316	-4.177	H
HETATM 1798	H	0	4.609	-12.479	-1.971	H	HETATM 1886	H	0	-4.892	9.358	-11.297	H
HETATM 1799	H	0	5.766	-5.472	-1.238	H	HETATM 1887	H	0	-5.058	8.563	-12.714	H
HETATM 1800	H	0	5.578	-3.572	-5.030	H	HETATM 1888	H	0	-1.348	5.399	-10.005	H
HETATM 1801	H	0	-2.805	-15.902	-3.519	H	HETATM 1889	H	0	-5.390	0.018	-2.112	H
HETATM 1802	H	0	-2.056	-15.384	-4.875	H	HETATM 1890	H	0	-5.912	-7.521	9.069	H
HETATM 1803	H	0	0.735	-13.446	-2.028	H	HETATM 1891	H	0	-3.983	-4.771	10.853	H
HETATM 1804	H	0	2.922	-13.023	-2.966	H	HETATM 1892	H	0	-3.495	-7.076	12.409	H
HETATM 1805	H	0	1.560	-10.348	-8.796	H	HETATM 1893	H	0	-6.895	-11.419	10.251	H
HETATM 1806	H	0	1.202	-11.320	-10.059	H	HETATM 1894	H	0	-6.975	-12.414	8.958	H
HETATM 1807	H	0	4.625	-10.483	-10.350	H	HETATM 1895	H	0	1.602	-9.078	7.307	H
HETATM 1808	H	0	3.481	-10.943	-11.421	H	HETATM 1896	H	0	5.264	4.973	-9.132	H
HETATM 1809	H	0	1.787	-4.963	-5.799	H	HETATM 1897	H	0	4.013	7.671	-12.167	H
HETATM 1810	H	0	4.077	-5.795	-5.963	H	HETATM 1898	H	0	5.020	-1.792	-14.481	H
HETATM 1811	H	0	4.685	-3.206	-2.457	H	HETATM 1899	H	0	3.526	-2.657	-14.520	H
HETATM 1812	H	0	-13.868	-9.487	-7.446	H	HETATM 1900	H	0	2.183	-3.058	-9.018	H
HETATM 1813	H	0	-15.920	-8.964	-5.650	H	HETATM 1901	H	0	3.302	-0.735	-8.251	H
HETATM 1814	H	0	-17.156	-6.847	-6.622	H	HETATM 1902	H	0	0.117	2.642	-13.671	H
HETATM 1815	H	0	-16.592	-5.453	-4.513	H	HETATM 1903	H	0	-1.412	2.688	-13.101	H
HETATM 1816	H	0	-14.077	-1.607	-4.052	H	HETATM 1904	H	0	1.895	1.188	-9.435	H
HETATM 1817	H	0	-10.353	-2.337	-6.423	H	HETATM 1905	H	0	1.201	5.462	-8.886	H
HETATM 1818	H	0	-7.774	0.100	-3.610	H	HETATM 1906	H	0	10.757	7.680	-8.940	H
HETATM 1819	H	0	-5.315	2.296	-6.541	H	HETATM 1907	H	0	10.478	4.357	-5.381	H
HETATM 1820	H	0	-1.347	3.402	-4.523	H	HETATM 1908	H	0	13.010	4.844	-6.482	H
HETATM 1821	H	0	-1.474	1.158	-2.655	H	HETATM 1909	H	0	11.805	1.769	-9.172	H
HETATM 1822	H	0	-3.068	-0.252	-3.885	H	HETATM 1910	H	0	9.824	5.924	-9.267	H
HETATM 1823	H	0	18.682	-11.621	-1.640	H	HETATM 1911	H	0	13.904	2.518	-7.072	H
HETATM 1824	H	0	-18.982	-1.019	-7.838	H	HETATM 1912	H	0	16.515	-1.167	-5.356	H
HETATM 1825	H	0	-19.897	-1.491	-9.106	H	HETATM 1913	H	0	15.137	-2.038	-5.452	H
HETATM 1826	H	0	-17.747	-0.369	-10.535	H	HETATM 1914	H	0	17.592	-0.641	-7.249	H
HETATM 1827	H	0	-19.008	-1.350	-10.872	H	HETATM 1915	H	0	16.873	-0.990	-8.673	H
HETATM 1828	H	0	-17.455	3.048	-10.038	H	HETATM 1916	H	0	-4.037	-14.757	-0.511	H
HETATM 1829	H	0	-18.051	1.647	-10.627	H	HETATM 1917	H	0	-1.463	-17.072	-0.149	H
HETATM 1830	H	0	-14.746	1.412	-9.168	H	HETATM 1918	H	0	-2.815	-17.566	-0.921	H
HETATM 1831	H	0	-15.357	0.638	-10.470	H	HETATM 1919	H	0	-4.196	-16.233	-1.190	H
HETATM 1832	H	0	-16.825	1.018	-7.364	H	HETATM 1920	H	0	0.291	-11.616	-0.006	H
HETATM 1833	H	0	-16.959	-2.693	-7.851	H	HETATM 1921	H	0	6.291	-9.017	2.453	H
HETATM 1834	H	0	-19.058	3.303	-3.458	H	HETATM 1922	H	0	0.309	-9.183	-1.605	H
HETATM 1835	H	0	-13.513	-4.892	-7.290	H	HETATM 1923	H	0	-3.946	-9.489	-0.937	H
HETATM 1836	H	0	-11.348	-3.420	-11.025	H	HETATM 1924	H	0	-1.914	-8.566	2.696	H
HETATM 1837	H	0	-19.850	1.576	-2.256	H	HETATM 1925	H	0	-2.436	-9.196	5.336	H
HETATM 1838	H	0	-18.227	4.929	-1.400	H	HETATM 1926	H	0	0.901	-13.607	7.204	H
HETATM 1839	H	0	-23.262	-1.037	2.024	H	HETATM 1927	H	0	-0.592	-14.145	7.591	H
HETATM 1840	H	0	-14.495	1.726	-4.133	H	HETATM 1928	H	0	-0.417	-10.453	6.257	H

HETATM 1929	H	0	7.331	-3.699	12.275	H	HETATM 1984	O	0	5.659	16.045	6.505	O
HETATM 1930	H	0	7.028	-4.593	9.813	H	HETATM 1985	H	0	6.395	15.271	6.252	H
HETATM 1931	H	0	10.090	-6.306	7.098	H	HETATM 1986	C	0	3.004	16.964	3.032	C
HETATM 1932	H	0	7.827	-0.598	9.123	H	HETATM 1987	H	0	2.402	16.705	2.153	H
HETATM 1933	H	0	9.291	2.691	6.992	H	HETATM 1988	H	0	2.381	16.877	3.924	H
HETATM 1934	H	0	10.239	-1.582	7.727	H	HETATM 1989	C	0	3.571	18.402	2.933	C
HETATM 1935	H	0	18.634	7.439	3.554	H	HETATM 1990	H	0	4.509	18.440	3.497	H
HETATM 1936	H	0	12.576	4.930	-1.740	H	HETATM 1991	H	0	3.810	18.643	1.887	H
HETATM 1937	H	0	10.569	6.801	-1.258	H	HETATM 1992	C	0	2.598	19.435	3.539	C
HETATM 1938	H	0	8.940	5.171	0.262	H	HETATM 1993	H	0	1.689	19.525	2.929	H
HETATM 1939	H	0	10.505	4.927	2.512	H	HETATM 1994	H	0	2.296	19.084	4.532	H
HETATM 1940	H	0	11.251	3.001	-3.185	H	HETATM 1995	C	0	3.278	20.815	3.681	C
HETATM 1941	H	0	13.482	-2.218	10.147	H	HETATM 1996	H	0	3.587	21.204	2.707	H
HETATM 1942	H	0	12.833	-2.850	8.788	H	HETATM 1997	H	0	4.195	20.717	4.268	H
HETATM 1943	H	0	12.038	-2.340	5.476	H	HETATM 1998	C	0	2.462	21.958	5.743	C
HETATM 1944	H	0	9.764	-6.981	4.800	H	HETATM 1999	C	0	1.588	22.643	3.541	C
HETATM 1945	H	0	10.266	-8.449	4.290	H	HETATM 2000	C	0	3.216	21.089	6.550	C
HETATM 1946	H	0	6.544	-2.603	6.806	H	HETATM 2001	C	0	1.708	23.031	6.358	C
HETATM 1947	H	0	10.074	-5.543	2.915	H	HETATM 2002	C	0	0.838	23.702	4.173	C
HETATM 1948	H	0	14.359	1.615	7.984	H	HETATM 2003	C	0	1.478	22.458	2.147	C
HETATM 1949	H	0	12.469	-3.840	2.823	H	HETATM 2004	C	0	3.288	21.268	7.965	C
HETATM 1950	H	0	8.519	-4.849	-1.571	H	HETATM 2005	H	0	3.734	20.246	6.121	H
HETATM 1951	H	0	8.607	-2.724	0.140	H	HETATM 2006	C	0	1.783	23.189	7.781	C
HETATM 1952	H	0	-2.796	-2.871	0.406	H	HETATM 2007	C	0	0.926	23.878	5.564	C
HETATM 1953	H	0	1.236	-3.014	-7.261	H	HETATM 2008	C	0	0.021	24.544	3.354	C
HETATM 1954	H	0	-1.217	-6.953	-2.237	H	HETATM 2009	H	0	2.002	21.648	1.666	H
HETATM 1955	H	0	7.413	4.134	6.280	H	HETATM 2010	C	0	0.666	23.308	1.346	C
HETATM 1956	H	0	-2.218	2.613	4.514	H	HETATM 2011	C	0	2.541	22.355	8.565	C
HETATM 1957	H	0	-0.865	2.206	6.974	H	HETATM 2012	H	0	1.219	23.998	8.238	H
HETATM 1958	H	0	-4.050	-0.569	7.626	H	HETATM 2013	H	0	0.366	24.682	6.035	H
HETATM 1959	H	0	-2.010	-2.482	7.834	H	HETATM 2014	C	0	-0.069	24.371	1.993	C
HETATM 1960	H	0	-2.416	-2.844	10.420	H	HETATM 2015	H	0	-0.538	25.343	3.836	H
HETATM 1961	H	0	0.030	6.103	2.342	H	HETATM 2016	H	0	2.575	22.513	9.635	H
HETATM 1962	H	0	-0.837	6.606	4.918	H	HETATM 2017	H	0	-0.696	25.035	1.411	H
HETATM 1963	H	0	-1.783	7.209	0.845	H	HETATM 2018	N	0	2.414	21.832	4.339	N
HETATM 1964	H	0	-0.955	10.227	7.427	H	HETATM 2019	N	0	4.042	20.438	8.751	N
HETATM 1965	H	0	-2.067	9.767	6.323	H	HETATM 2020	N	0	0.573	23.130	-0.016	N
HETATM 1966	H	0	-3.014	5.001	4.929	H	HETATM 2021	C	0	1.345	22.069	-0.684	C
HETATM 1967	H	0	-1.748	9.913	1.585	H	HETATM 2022	H	0	1.171	22.115	-1.760	H
HETATM 1968	H	0	-0.906	12.242	-6.467	H	HETATM 2023	H	0	2.424	22.190	-0.512	H
HETATM 1969	H	0	0.453	12.807	-4.097	H	HETATM 2024	H	0	1.043	21.070	-0.335	H
HETATM 1970	H	0	2.957	10.175	-1.084	H	HETATM 2025	C	0	-0.290	24.004	-0.837	C
HETATM 1971	H	0	1.179	10.597	0.817	H	HETATM 2026	H	0	0.038	25.051	-0.794	H
HETATM 1972	H	0	3.290	13.159	-0.341	H	HETATM 2027	H	0	-0.242	23.679	-1.878	H
HETATM 1973	C	0	6.973	14.058	4.492	C	HETATM 2028	H	0	-1.338	23.948	-0.515	H
HETATM 1974	O	0	7.648	13.279	3.711	O	HETATM 2029	C	0	4.855	19.357	8.149	C
HETATM 1975	O	0	7.234	14.331	5.720	O	HETATM 2030	H	0	5.637	19.773	7.497	H
HETATM 1976	C	0	5.786	14.699	3.846	C	HETATM 2031	H	0	5.344	18.788	8.941	H
HETATM 1977	C	0	4.905	15.702	4.250	C	HETATM 2032	H	0	4.248	18.660	7.562	H
HETATM 1978	N	0	5.502	14.336	2.530	N	HETATM 2033	C	0	4.106	20.632	10.214	C
HETATM 1979	C	0	4.479	15.109	2.129	C	HETATM 2034	H	0	4.740	19.857	10.647	H
HETATM 1980	H	0	4.040	15.110	1.145	H	HETATM 2035	H	0	4.538	21.608	10.475	H
HETATM 1981	N	0	4.080	15.947	3.138	N	HETATM 2036	H	0	3.113	20.550	10.674	H
HETATM 1982	C	0	4.797	16.416	5.563	C	END						
HETATM 1983	O	0	3.933	17.318	5.729	O							

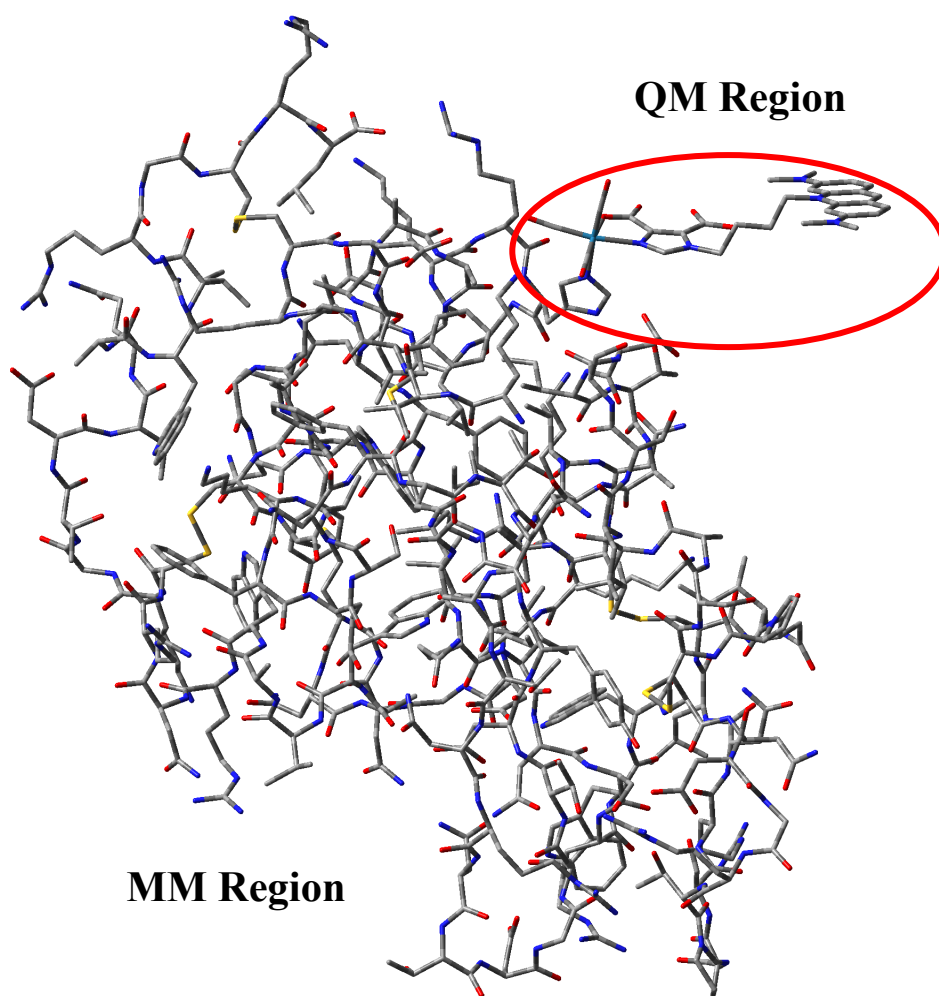


Figure S2. QM/MM optimized structure of Lys2.

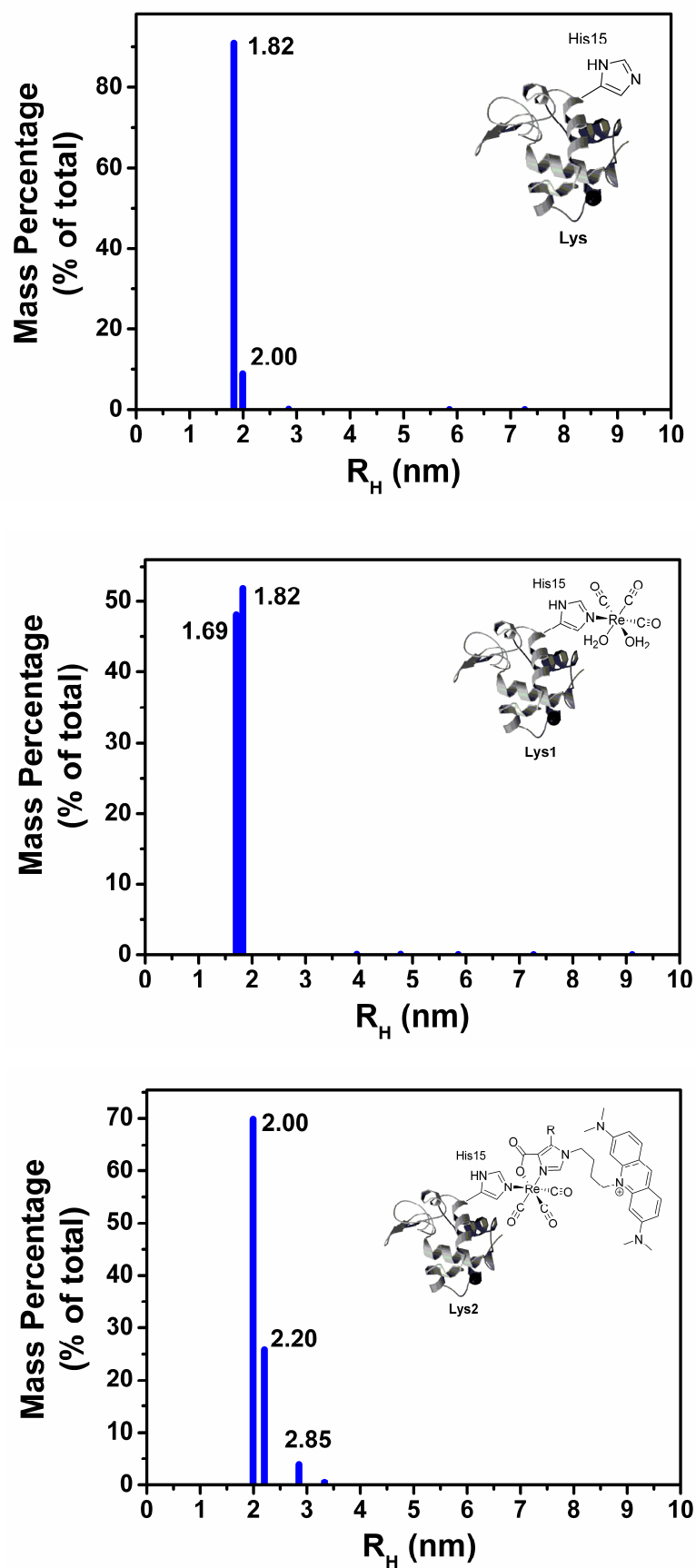


Figure S3. Dynamic light scattering (DLS) of an aqueous solution of (from top to bottom) Lys, Lys1 and Lys2.

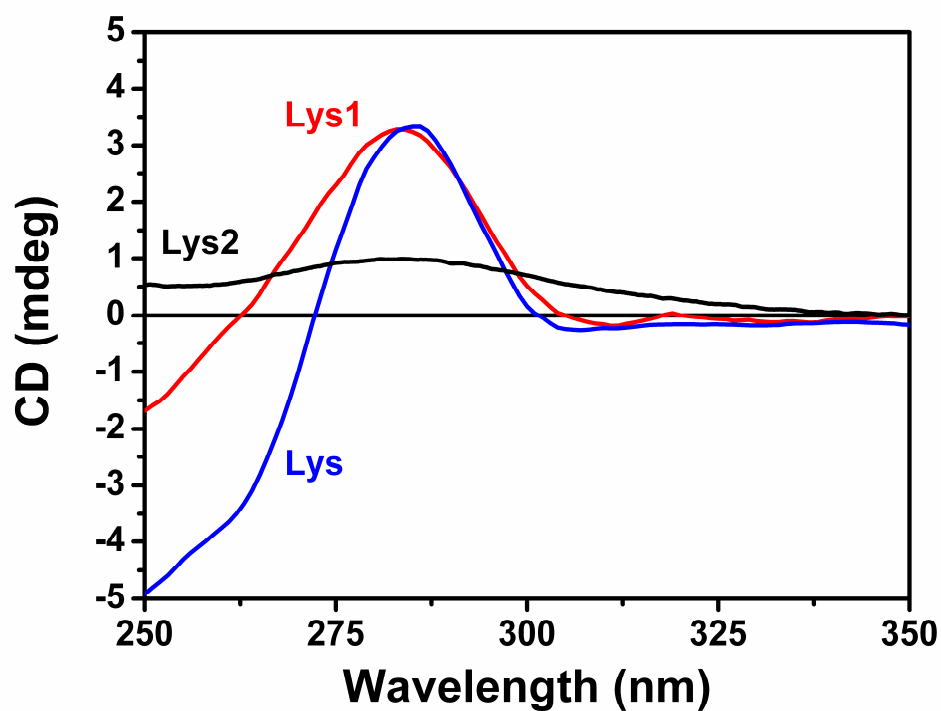


Figure S4. Circular dichroism (CD) spectra of Lys, Lys1 and Lys2. Samples were recorded in a 50mM ammonium acetate buffer (pH 4.6) in 0.9M NaCl.

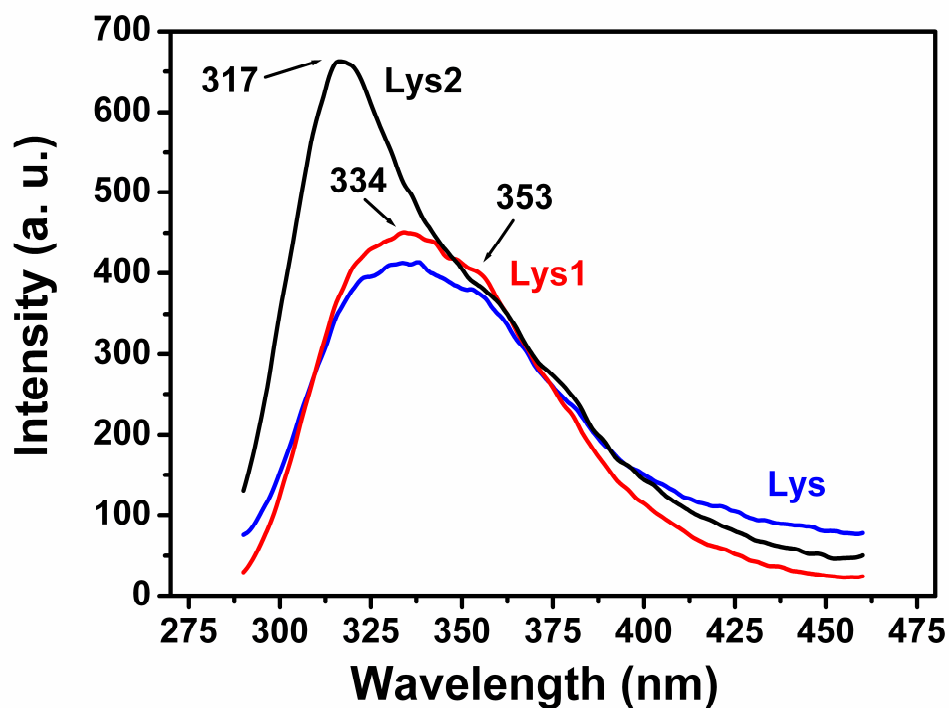


Figure S5. Intrinsic fluorescence spectra of Lys, Lys1 and Lys2.