Supporting Information for

Clotrimazole-cyclodextrin based approach for the management and treatment of *Candidiasis- A formulation and chemistry based evaluation*

Table S1. Energies, thermodynamics and electronic properties of the optimized geometry of free clotrimazole, HPCD and clotrimazole–HPCD using B3LYP/6-31G(d,p) and single point energy calculation using B3LYP/6-311G+(d,p).

Properties	**Clotrimazole (CT)**	**HPCD (Lowest Energy Conformer)**	**CT–HPCD (Inclusion Complex)**
E(B3LYP) (kcal/mol)	–889,979.781	–3,531,321.630	–4,421,324.010
H° (kcal/mol)	–889,757.643	–3,530,091.090	–4,419,870.690
G° (kcal/mol)	–889,801.568	–3,530,250.480	–4,420,056.440
S° (cal mol^{-1} K^{-1})	145.420	534.308	625.706
Single point energy (SPE) (kcal/mol)	–890,130.383	–3,532,293.650	–4,422,433.442

The xyz-coordinates (in pdb format) of the HPCD: CT complex, which was optimized using hybrid density functional theory (DFT) B3LYP/6-31G(d, p), is as follows:

COMPND HPCD:CT optimized complex using hybrid density functional theory (DFT) B3LYP/6-31G(d,p)

HETATM 1 C LIG 1 4.916 -3.146 -2.079 1.00 0.00 C

HETATM 2 C LIG 1 5.669 -3.226 -0.746 1.00 0.00 C

HETATM 3 O LIG 1 5.422 -4.424 -0.033 1.00 0.00 O

HETATM 4 C LIG 1 5.333 -2.008 0.123 1.00 0.00 C

HETATM 5 O LIG 1 6.137 -2.047 1.298 1.00 0.00 O

HETATM 6 C LIG 1 5.571 -0.697 -0.626 1.00 0.00 C

HETATM 7 O LIG 1 5.118 0.387 0.202 1.00 0.00 O

HETATM 8 C LIG 1 4.763 -0.744 -1.942 1.00 0.00 C

HETATM 9 O LIG 1 5.167 -1.907 -2.701 1.00 0.00 O

HETATM 10 C LIG 1 4.935 0.457 -2.882 1.00 0.00 C

HETATM 11 C LIG 1 6.035 1.389 0.608 1.00 0.00 C

HETATM 12 C LIG 1 6.183 1.408 2.139 1.00 0.00 C

HETATM 13 O LIG 1 6.691 0.226 2.711 1.00 0.00 O

HETATM 14 C LIG 1 4.842 1.785 2.771 1.00 0.00 C

HETATM 15 O LIG 1 4.967 1.851 4.186 1.00 0.00 O

HETATM 16 C LIG 1 4.387 3.144 2.268 1.00 0.00 C

HETATM 17 O LIG 1 3.072 3.368 2.777 1.00 0.00 O

HETATM 18 C LIG 1 4.380 3.194 0.727 1.00 0.00 C

HETATM	19	O	LIG	1	5.612	2.674	0.180	1.00	0.00	O
HETATM	20	C	LIG	1	4.257	4.632	0.231	1.00	0.00	C
HETATM	21	O	LIG	1	4.055	4.661	-1.176	1.00	0.00	O
HETATM	22	C	LIG	1	2.785	4.570	3.466	1.00	0.00	C
HETATM	23	C	LIG	1	2.163	4.207	4.820	1.00	0.00	C
HETATM	24	O	LIG	1	2.983	3.395	5.635	1.00	0.00	O
HETATM	25	C	LIG	1	0.801	3.549	4.591	1.00	0.00	C
HETATM	26	O	LIG	1	0.163	3.304	5.842	1.00	0.00	O
HETATM	27	C	LIG	1	-0.099	4.442	3.746	1.00	0.00	C
HETATM	28	O	LIG	1	-1.295	3.708	3.482	1.00	0.00	O
HETATM	29	C	LIG	1	0.619	4.812	2.432	1.00	0.00	C
HETATM	30	O	LIG	1	1.907	5.390	2.730	1.00	0.00	O
HETATM	31	C	LIG	1	-0.135	5.837	1.602	1.00	0.00	C
HETATM	32	O	LIG	1	0.380	5.825	0.280	1.00	0.00	O
HETATM	33	C	LIG	1	-2.550	4.272	3.813	1.00	0.00	C
HETATM	34	C	LIG	1	-3.305	3.287	4.713	1.00	0.00	C
HETATM	35	O	LIG	1	-2.664	2.984	5.935	1.00	0.00	O
HETATM	36	C	LIG	1	-3.581	2.007	3.927	1.00	0.00	C
HETATM	37	O	LIG	1	-4.362	1.118	4.738	1.00	0.00	O
HETATM	38	C	LIG	1	-4.327	2.296	2.629	1.00	0.00	C
HETATM	39	O	LIG	1	-4.361	1.109	1.830	1.00	0.00	O

HETATM	40	C	LIG	1	-3.599	3.395	1.828	1.00	0.00	C
HETATM	41	O	LIG	1	-3.319	4.535	2.663	1.00	0.00	O
HETATM	42	C	LIG	1	-4.446	3.915	0.667	1.00	0.00	C
HETATM	43	O	LIG	1	-3.736	4.772	-0.201	1.00	0.00	O
HETATM	44	C	LIG	1	-5.537	0.332	1.826	1.00	0.00	C
HETATM	45	C	LIG	1	-5.207	-1.126	2.183	1.00	0.00	C
HETATM	46	O	LIG	1	-4.511	-1.307	3.401	1.00	0.00	O
HETATM	47	C	LIG	1	-4.353	-1.738	1.074	1.00	0.00	C
HETATM	48	O	LIG	1	-4.073	-3.104	1.361	1.00	0.00	O
HETATM	49	C	LIG	1	-5.049	-1.646	-0.281	1.00	0.00	C
HETATM	50	O	LIG	1	-4.140	-2.116	-1.276	1.00	0.00	O
HETATM	51	C	LIG	1	-5.399	-0.167	-0.548	1.00	0.00	C
HETATM	52	O	LIG	1	-6.169	0.363	0.558	1.00	0.00	O
HETATM	53	C	LIG	1	-6.234	0.043	-1.801	1.00	0.00	C
HETATM	54	O	LIG	1	-6.296	1.436	-2.090	1.00	0.00	O
HETATM	55	C	LIG	1	-4.568	-3.120	-2.199	1.00	0.00	C
HETATM	56	C	LIG	1	-4.317	-4.550	-1.679	1.00	0.00	C
HETATM	57	O	LIG	1	-5.069	-4.844	-0.525	1.00	0.00	O
HETATM	58	C	LIG	1	-2.807	-4.768	-1.500	1.00	0.00	C
HETATM	59	O	LIG	1	-2.490	-6.111	-1.153	1.00	0.00	O
HETATM	60	C	LIG	1	-2.055	-4.419	-2.788	1.00	0.00	C

HETATM	61	O	LIG	1	-0.657	-4.443	-2.491	1.00	0.00	O
HETATM	62	C	LIG	1	-2.439	-3.013	-3.288	1.00	0.00	C
HETATM	63	O	LIG	1	-3.873	-2.913	-3.403	1.00	0.00	O
HETATM	64	C	LIG	1	-1.841	-2.656	-4.649	1.00	0.00	C
HETATM	65	O	LIG	1	-1.644	-1.251	-4.817	1.00	0.00	O
HETATM	66	C	LIG	1	0.176	-5.376	-3.142	1.00	0.00	C
HETATM	67	C	LIG	1	1.030	-6.084	-2.080	1.00	0.00	C
HETATM	68	O	LIG	1	0.276	-6.710	-1.060	1.00	0.00	O
HETATM	69	C	LIG	1	1.998	-5.080	-1.453	1.00	0.00	C
HETATM	70	O	LIG	1	2.917	-5.741	-0.584	1.00	0.00	O
HETATM	71	C	LIG	1	2.810	-4.343	-2.508	1.00	0.00	C
HETATM	72	O	LIG	1	3.541	-3.328	-1.814	1.00	0.00	O
HETATM	73	C	LIG	1	1.872	-3.731	-3.565	1.00	0.00	C
HETATM	74	O	LIG	1	1.008	-4.752	-4.098	1.00	0.00	O
HETATM	75	C	LIG	1	2.631	-3.122	-4.728	1.00	0.00	C
HETATM	76	O	LIG	1	1.736	-2.366	-5.523	1.00	0.00	O
HETATM	77	H	LIG	1	5.279	-3.910	-2.776	1.00	0.00	H
HETATM	78	H	LIG	1	6.744	-3.200	-0.963	1.00	0.00	H
HETATM	79	H	LIG	1	4.269	-2.050	0.394	1.00	0.00	H
HETATM	80	H	LIG	1	6.048	-2.945	1.654	1.00	0.00	H
HETATM	81	H	LIG	1	6.641	-0.580	-0.844	1.00	0.00	H

HETATM	82	H	LIG	1	3.702	-0.837	-1.685	1.00	0.00	H
HETATM	83	H	LIG	1	5.352	1.323	-2.353	1.00	0.00	H
HETATM	84	H	LIG	1	5.638	0.171	-3.669	1.00	0.00	H
HETATM	85	H	LIG	1	7.006	1.230	0.128	1.00	0.00	H
HETATM	86	H	LIG	1	6.907	2.198	2.374	1.00	0.00	H
HETATM	87	H	LIG	1	4.088	1.035	2.494	1.00	0.00	H
HETATM	88	H	LIG	1	5.494	1.075	4.437	1.00	0.00	H
HETATM	89	H	LIG	1	5.075	3.906	2.661	1.00	0.00	H
HETATM	90	H	LIG	1	3.536	2.599	0.357	1.00	0.00	H
HETATM	91	H	LIG	1	3.408	5.111	0.735	1.00	0.00	H
HETATM	92	H	LIG	1	5.175	5.171	0.502	1.00	0.00	H
HETATM	93	H	LIG	1	3.698	5.159	3.605	1.00	0.00	H
HETATM	94	H	LIG	1	2.003	5.141	5.372	1.00	0.00	H
HETATM	95	H	LIG	1	0.949	2.603	4.051	1.00	0.00	H
HETATM	96	H	LIG	1	0.841	2.905	6.409	1.00	0.00	H
HETATM	97	H	LIG	1	-0.334	5.356	4.311	1.00	0.00	H
HETATM	98	H	LIG	1	0.752	3.901	1.836	1.00	0.00	H
HETATM	99	H	LIG	1	-1.209	5.605	1.594	1.00	0.00	H
HETATM	100	H	LIG	1	0.004	6.827	2.064	1.00	0.00	H
HETATM	101	H	LIG	1	-2.419	5.236	4.315	1.00	0.00	H
HETATM	102	H	LIG	1	-4.265	3.751	4.972	1.00	0.00	H

HETATM 103 H LIG 1 -2.625 1.530 3.672 1.00 0.00 H

HETATM 104 H LIG 1 -4.003 1.212 5.637 1.00 0.00 H

HETATM 105 H LIG 1 -5.349 2.625 2.864 1.00 0.00 H

HETATM 106 H LIG 1 -2.658 2.977 1.451 1.00 0.00 H

HETATM 107 H LIG 1 -4.878 3.064 0.125 1.00 0.00 H

HETATM 108 H LIG 1 -5.265 4.510 1.088 1.00 0.00 H

HETATM 109 H LIG 1 -6.273 0.745 2.525 1.00 0.00 H

HETATM 110 H LIG 1 -6.167 -1.664 2.223 1.00 0.00 H

HETATM 111 H LIG 1 -3.412 -1.175 1.019 1.00 0.00 H

HETATM 112 H LIG 1 -3.853 -3.189 2.303 1.00 0.00 H

HETATM 113 H LIG 1 -5.959 -2.258 -0.269 1.00 0.00 H

HETATM 114 H LIG 1 -4.467 0.401 -0.645 1.00 0.00 H

HETATM 115 H LIG 1 -5.758 -0.490 -2.635 1.00 0.00 H

HETATM 116 H LIG 1 -7.236 -0.370 -1.641 1.00 0.00 H

HETATM 117 H LIG 1 -5.632 -2.989 -2.430 1.00 0.00 H

HETATM 118 H LIG 1 -4.674 -5.233 -2.459 1.00 0.00 H

HETATM 119 H LIG 1 -2.451 -4.085 -0.719 1.00 0.00 H

HETATM 120 H LIG 1 -2.693 -6.240 -0.198 1.00 0.00 H

HETATM 121 H LIG 1 -2.291 -5.169 -3.557 1.00 0.00 H

HETATM 122 H LIG 1 -2.072 -2.278 -2.563 1.00 0.00 H

HETATM 123 H LIG 1 -0.849 -3.101 -4.748 1.00 0.00 H

HETATM 124 H LIG 1 -2.491 -3.053 -5.443 1.00 0.00 H

HETATM 125 H LIG 1 -0.423 -6.101 -3.703 1.00 0.00 H

HETATM 126 H LIG 1 1.622 -6.852 -2.596 1.00 0.00 H

HETATM 127 H LIG 1 1.412 -4.337 -0.894 1.00 0.00 H

HETATM 128 H LIG 1 2.392 -6.254 0.050 1.00 0.00 H

HETATM 129 H LIG 1 3.504 -5.049 -2.986 1.00 0.00 H

HETATM 130 H LIG 1 1.273 -2.947 -3.088 1.00 0.00 H

HETATM 131 H LIG 1 3.423 -2.476 -4.328 1.00 0.00 H

HETATM 132 H LIG 1 3.101 -3.923 -5.323 1.00 0.00 H

HETATM 133 H LIG 1 4.496 -4.705 -0.184 1.00 0.00 H

HETATM 134 H LIG 1 6.306 -0.561 2.269 1.00 0.00 H

HETATM 135 H LIG 1 3.467 2.750 5.081 1.00 0.00 H

HETATM 136 H LIG 1 -1.695 2.927 5.796 1.00 0.00 H

HETATM 137 H LIG 1 -4.509 -0.484 3.932 1.00 0.00 H

HETATM 138 H LIG 1 -4.699 -4.339 0.225 1.00 0.00 H

HETATM 139 H LIG 1 -0.672 -6.453 -1.132 1.00 0.00 H

HETATM 140 C LIG 1 -7.563 1.929 -2.532 1.00 0.00 C

HETATM 141 C LIG 1 -8.417 2.440 -1.367 1.00 0.00 C

HETATM 142 C LIG 1 -9.755 2.981 -1.857 1.00 0.00 C

HETATM 143 O LIG 1 -8.693 1.403 -0.433 1.00 0.00 O

HETATM 144 C LIG 1 -2.922 4.131 -1.186 1.00 0.00 C

HETATM	145	C	LIG	1	-3.161	4.790	-2.551	1.00	0.00	C
HETATM	146	C	LIG	1	-4.616	4.660	-3.003	1.00	0.00	C
HETATM	147	C	LIG	1	-0.005	6.972	-0.472	1.00	0.00	C
HETATM	148	C	LIG	1	0.481	6.794	-1.907	1.00	0.00	C
HETATM	149	C	LIG	1	0.180	8.024	-2.754	1.00	0.00	C
HETATM	150	O	LIG	1	1.891	6.591	-1.945	1.00	0.00	O
HETATM	151	C	LIG	1	4.889	5.528	-1.967	1.00	0.00	C
HETATM	152	C	LIG	1	5.674	4.696	-2.979	1.00	0.00	C
HETATM	153	O	LIG	1	6.562	3.797	-2.326	1.00	0.00	O
HETATM	154	C	LIG	1	6.504	5.577	-3.905	1.00	0.00	C
HETATM	155	O	LIG	1	3.716	0.810	-3.522	1.00	0.00	O
HETATM	156	C	LIG	1	2.916	1.675	-2.719	1.00	0.00	C
HETATM	157	C	LIG	1	1.616	2.037	-3.426	1.00	0.00	C
HETATM	158	C	LIG	1	0.940	3.200	-2.712	1.00	0.00	C
HETATM	159	O	LIG	1	0.716	0.917	-3.449	1.00	0.00	O
HETATM	160	C	LIG	1	2.392	-1.405	-6.337	1.00	0.00	C
HETATM	161	C	LIG	1	1.321	-0.576	-7.033	1.00	0.00	C
HETATM	162	C	LIG	1	1.927	0.533	-7.883	1.00	0.00	C
HETATM	163	O	LIG	1	0.467	0.029	-6.059	1.00	0.00	O
HETATM	164	H	LIG	1	-9.616	3.803	-2.568	1.00	0.00	H
HETATM	165	H	LIG	1	-10.330	2.188	-2.347	1.00	0.00	H

HETATM	166	H	LIG	1	-10.341	3.348	-1.011	1.00	0.00	H
HETATM	167	H	LIG	1	-7.859	1.167	0.006	1.00	0.00	H
HETATM	168	H	LIG	1	-1.863	4.224	-0.915	1.00	0.00	H
HETATM	169	H	LIG	1	-3.165	3.060	-1.260	1.00	0.00	H
HETATM	170	H	LIG	1	-4.745	5.115	-3.989	1.00	0.00	H
HETATM	171	H	LIG	1	-4.910	3.606	-3.059	1.00	0.00	H
HETATM	172	H	LIG	1	-1.100	7.090	-0.459	1.00	0.00	H
HETATM	173	H	LIG	1	0.446	7.876	-0.030	1.00	0.00	H
HETATM	174	H	LIG	1	-0.896	8.219	-2.797	1.00	0.00	H
HETATM	175	H	LIG	1	0.684	8.906	-2.345	1.00	0.00	H
HETATM	176	H	LIG	1	2.107	5.824	-1.393	1.00	0.00	H
HETATM	177	H	LIG	1	6.103	3.422	-1.556	1.00	0.00	H
HETATM	178	H	LIG	1	7.081	4.951	-4.590	1.00	0.00	H
HETATM	179	H	LIG	1	5.866	6.242	-4.496	1.00	0.00	H
HETATM	180	H	LIG	1	7.209	6.185	-3.328	1.00	0.00	H
HETATM	181	H	LIG	1	2.664	1.195	-1.759	1.00	0.00	H
HETATM	182	H	LIG	1	3.477	2.590	-2.490	1.00	0.00	H
HETATM	183	H	LIG	1	-0.013	3.447	-3.180	1.00	0.00	H
HETATM	184	H	LIG	1	0.748	2.952	-1.661	1.00	0.00	H
HETATM	185	H	LIG	1	0.867	0.441	-4.291	1.00	0.00	H
HETATM	186	H	LIG	1	3.039	-1.897	-7.082	1.00	0.00	H

HETATM 187 H LIG 1 1.135 1.111 -8.366 1.00 0.00 H

HETATM 188 H LIG 1 2.514 1.215 -7.259 1.00 0.00 H

HETATM 189 H LIG 1 2.582 0.122 -8.657 1.00 0.00 H

HETATM 190 H LIG 1 -0.177 -0.633 -5.730 1.00 0.00 H

HETATM 191 H LIG 1 1.853 2.328 -4.459 1.00 0.00 H

HETATM 192 H LIG 1 1.575 4.089 -2.738 1.00 0.00 H

HETATM 193 H LIG 1 3.016 -0.746 -5.714 1.00 0.00 H

HETATM 194 H LIG 1 0.723 -1.245 -7.669 1.00 0.00 H

HETATM 195 H LIG 1 4.941 4.135 -3.583 1.00 0.00 H

HETATM 196 C LIG 1 -2.839 -0.484 -5.025 1.00 0.00 C

HETATM 197 C LIG 1 -2.501 1.004 -5.056 1.00 0.00 C

HETATM 198 O LIG 1 -2.081 1.456 -3.763 1.00 0.00 O

HETATM 199 C LIG 1 -3.733 1.811 -5.457 1.00 0.00 C

HETATM 200 H LIG 1 -3.305 -0.790 -5.974 1.00 0.00 H

HETATM 201 H LIG 1 -3.548 -0.675 -4.215 1.00 0.00 H

HETATM 202 H LIG 1 -1.137 1.220 -3.627 1.00 0.00 H

HETATM 203 H LIG 1 -3.493 2.877 -5.466 1.00 0.00 H

HETATM 204 H LIG 1 -4.085 1.523 -6.453 1.00 0.00 H

HETATM 205 H LIG 1 -0.039 5.925 -2.337 1.00 0.00 H

HETATM 206 H LIG 1 0.541 7.868 -3.774 1.00 0.00 H

HETATM 207 H LIG 1 -5.280 5.163 -2.294 1.00 0.00 H

HETATM	208	O	LIG	1	-2.247	4.271	-3.508	1.00	0.00	O
HETATM	209	H	LIG	1	-2.916	5.856	-2.457	1.00	0.00	H
HETATM	210	H	LIG	1	-2.304	3.292	-3.528	1.00	0.00	H
HETATM	211	H	LIG	1	-7.854	3.252	-0.878	1.00	0.00	H
HETATM	212	H	LIG	1	-1.697	1.169	-5.785	1.00	0.00	H
HETATM	213	H	LIG	1	-4.544	1.650	-4.738	1.00	0.00	H
HETATM	214	H	LIG	1	4.237	6.250	-2.470	1.00	0.00	H
HETATM	215	H	LIG	1	5.589	6.073	-1.320	1.00	0.00	H
HETATM	216	H	LIG	1	-7.348	2.750	-3.225	1.00	0.00	H
HETATM	217	H	LIG	1	-8.111	1.151	-3.082	1.00	0.00	H
HETATM	218	CL	LIG	2	2.665	-1.758	3.429	1.00	0.00	Cl
HETATM	219	N	LIG	2	-1.077	-4.596	2.921	1.00	0.00	N
HETATM	220	N	LIG	2	-2.301	-6.024	1.717	1.00	0.00	N
HETATM	221	C	LIG	2	0.122	-3.762	3.284	1.00	0.00	C
HETATM	222	C	LIG	2	0.348	-2.687	2.176	1.00	0.00	C
HETATM	223	C	LIG	2	-0.178	-2.989	4.598	1.00	0.00	C
HETATM	224	C	LIG	2	1.264	-4.804	3.404	1.00	0.00	C
HETATM	225	C	LIG	2	1.441	-1.795	2.155	1.00	0.00	C
HETATM	226	C	LIG	2	-0.610	-2.496	1.165	1.00	0.00	C
HETATM	227	C	LIG	2	0.579	-3.141	5.765	1.00	0.00	C
HETATM	228	C	LIG	2	1.128	-5.831	4.355	1.00	0.00	C

HETATM	229	C	LIG	2	-1.222	-2.048	4.603	1.00	0.00	C
HETATM	230	C	LIG	2	2.368	-4.845	2.548	1.00	0.00	C
HETATM	231	C	LIG	2	-2.277	-4.770	3.595	1.00	0.00	C
HETATM	232	C	LIG	2	-1.145	-5.394	1.812	1.00	0.00	C
HETATM	233	C	LIG	2	-3.011	-5.649	2.837	1.00	0.00	C
HETATM	234	C	LIG	2	1.614	-0.858	1.131	1.00	0.00	C
HETATM	235	C	LIG	2	-0.465	-1.545	0.157	1.00	0.00	C
HETATM	236	C	LIG	2	0.285	-2.397	6.911	1.00	0.00	C
HETATM	237	C	LIG	2	2.089	-6.831	4.478	1.00	0.00	C
HETATM	238	C	LIG	2	-1.520	-1.313	5.749	1.00	0.00	C
HETATM	239	C	LIG	2	3.338	-5.846	2.672	1.00	0.00	C
HETATM	240	C	LIG	2	0.668	-0.739	0.115	1.00	0.00	C
HETATM	241	C	LIG	2	-0.767	-1.485	6.911	1.00	0.00	C
HETATM	242	C	LIG	2	3.207	-6.837	3.642	1.00	0.00	C
HETATM	243	H	LIG	2	-1.512	-3.092	1.171	1.00	0.00	H
HETATM	244	H	LIG	2	1.415	-3.827	5.785	1.00	0.00	H
HETATM	245	H	LIG	2	0.253	-5.857	4.996	1.00	0.00	H
HETATM	246	H	LIG	2	-1.823	-1.884	3.715	1.00	0.00	H
HETATM	247	H	LIG	2	2.487	-4.103	1.769	1.00	0.00	H
HETATM	248	H	LIG	2	-2.487	-4.287	4.534	1.00	0.00	H
HETATM	249	H	LIG	2	-0.339	-5.482	1.099	1.00	0.00	H

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HETATM  250  H   LIG    2     -4.002  -6.031   3.034  1.00  0.00           H
HETATM  251  H   LIG    2      2.497  -0.230   1.138  1.00  0.00           H
HETATM  252  H   LIG    2     -1.246  -1.441  -0.588  1.00  0.00           H
HETATM  253  H   LIG    2      0.892  -2.533   7.802  1.00  0.00           H
HETATM  254  H   LIG    2      1.958  -7.610   5.223  1.00  0.00           H
HETATM  255  H   LIG    2     -2.341  -0.604   5.721  1.00  0.00           H
HETATM  256  H   LIG    2      4.196  -5.836   2.008  1.00  0.00           H
HETATM  257  H   LIG    2      0.806  -0.028  -0.694  1.00  0.00           H
HETATM  258  H   LIG    2     -0.994  -0.909   7.803  1.00  0.00           H
HETATM  259  H   LIG    2      3.960  -7.613   3.738  1.00  0.00           H
CONECT    1   77    9   72    2
CONECT    1
CONECT    2    1   78    3    4
CONECT    2
CONECT    3    2  133
CONECT    4    2    6   79    5
CONECT    4
CONECT    5    4   80
CONECT    6    8   81    4    7
CONECT    6
CONECT    7    6   11
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CONECT 8 10 9 82 6

CONECT 8

CONECT 9 1 8

CONECT 10 84 155 83 8

CONECT 10

CONECT 11 85 19 7 12

CONECT 11

CONECT 12 11 86 13 14

CONECT 12

CONECT 13 12 134

CONECT 14 12 16 87 15

CONECT 14

CONECT 15 14 88

CONECT 16 18 89 14 17

CONECT 16

CONECT 17 16 22

CONECT 18 19 20 90 16

CONECT 18

CONECT 19 11 18

CONECT 20 21 92 18 91

CONECT 20

CONECT 21 151 20

CONECT 22 30 17 93 23

CONECT 22

CONECT 23 22 25 94 24

CONECT 23

CONECT 24 23 135

CONECT 25 27 95 23 26

CONECT 25

CONECT 26 25 96

CONECT 27 29 28 97 25

CONECT 27

CONECT 28 27 33

CONECT 29 31 98 30 27

CONECT 29

CONECT 30 29 22

CONECT 31 32 99 100 29

CONECT 31

CONECT 32 147 31

CONECT 33 41 28 101 34

CONECT 33

CONECT 34 33 36 102 35

CONECT 34

CONECT 35 34 136

CONECT 36 38 103 34 37

CONECT 36

CONECT 37 36 104

CONECT 38 40 39 105 36

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CONECT 39 44 38

CONECT 40 42 106 38 41

CONECT 40

CONECT 41 40 33

CONECT 42 43 107 108 40

CONECT 42

CONECT 43 144 42

CONECT 44 52 39 45 109

CONECT 44

CONECT 45 47 44 110 46

CONECT 45

CONECT 46 45 137

CONECT 47 49 111 48 45

CONECT 47

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CONECT 63 62 55

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CONECT 66

CONECT 67 66 126 69 68

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CONECT 71

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CONECT 73

CONECT 74 73 66

CONECT 75 76 132 131 73

CONECT 75

CONECT 76 160 75

CONECT 77 1

CONECT 78 2

CONECT 79 4

CONECT 80 5

CONECT 81 6

CONECT 82 8

CONECT 83 10

CONECT 84 10

CONECT 85 11

CONECT 86 12

CONECT 87 14

CONECT 88 15

CONECT 89 16

CONECT 90 18

CONECT 91 20

CONECT 92 20

CONECT 93 22

CONECT 94 23

CONECT 95 25

CONECT 96 26

CONECT 97 27

CONECT 98 29

CONECT 99 31

CONECT 100 31

CONECT 101 33

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CONECT 107 42

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CONECT 123 64

CONECT 124 64

CONECT 125 66

CONECT 126 67

CONECT 127 69

CONECT 128 70

CONECT 129 71

CONECT 130 73

CONECT 131 75

CONECT 132 75

CONECT 133 3

CONECT 134 13

CONECT 135 24

CONECT 136 35

CONECT 137 46

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CONECT  140
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CONECT  141
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CONECT  144  145  169  168   43
CONECT  144
CONECT  145  208  146  209  144
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CONECT  146  170  171  145  207
CONECT  146
CONECT  147  148  172  173   32
CONECT  147
CONECT  148  149  205  150  147
CONECT  148
CONECT  149  206  174  175  148
CONECT  149
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CONECT 150 148 176

CONECT 151 152 214 215   21

CONECT 151

CONECT 152 154 195 153 151

CONECT 152

CONECT 153 152 177

CONECT 154 178 179 180 152

CONECT 154

CONECT 155   10 156

CONECT 156 155 157 182 181

CONECT 156

CONECT 157 191 159 156 158

CONECT 157

CONECT 158 157 183 192 184

CONECT 158

CONECT 159 185 157

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CONECT 160

CONECT 161 162 194 160 163

CONECT 161

CONECT 162 189 187 188 161

CONECT 162

CONECT 163 161 190

CONECT 164 142

CONECT 165 142

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CONECT 167 143

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CONECT 196 200 197 65 201

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CONECT 197 212 199 196 198

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CONECT 211 141

CONECT 212 197