Initial structure of OMP:

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generated by VMD

N	3.771554	0.837824	5.606754
N	-2.633097	6.048390	4.258596
N	2.308138	2.315110	6.503703
N	-1.169679	4.571104	3.361647
N	-0.979185	-0.345334	3.355810
N	2.117643	7.231548	6.509541
H	4.097772	-0.002745	5.087189
H	-2.959313	6.888959	4.778162
H	3.360426	4.699407	7.676131
H	-2.221968	2.186807	2.189220
H	-4.006973	5.096618	7.751964
H	5.145432	1.789596	2.113387
H	-3.231805	1.331531	5.755560
H	4.370263	5.554684	4.109790
H	1.374751	1.352085	3.288760
H	-0.236294	5.534128	6.576591
H	2.342208	-0.147995	3.371492
H	-1.203750	7.034207	6.493859
H	2.251932	8.659158	3.185429
H	-1.113474	-1.772943	6.679921
H	2.348159	-0.216661	0.921390
H	-1.209701	7.102875	8.943961
H	-2.719068	7.795626	0.054828
H	3.857526	-0.909412	9.810523

H	-2.026226	7.696866	1.690598
H	3.164684	-0.810653	8.174752
H	-1.936277	4.872894	9.617558
H	3.074735	2.013320	0.247793
H	1.237994	7.636951	1.276633
H	-0.099536	-0.750738	8.588717
H	2.153547	6.163002	0.920125
H	-1.015090	0.723211	8.945225
H	5.979829	5.504379	0.536457
H	-4.841370	1.381835	9.328894
H	1.190712	2.718915	8.750191
H	-0.052254	4.167297	1.115160
H	4.233587	5.173156	0.337997
H	-3.095129	1.713058	9.527353
H	-1.295226	1.688029	6.907297
H	2.433685	5.198184	2.958053
H	-0.220772	3.083862	6.599760
H	1.359230	3.802351	3.265590
H	-1.330849	2.508477	5.314569
H	2.469308	4.377736	4.550781
C	2.460806	1.177815	5.840623
C	-1.322347	5.708398	4.024727
C	3.600817	2.771921	6.697652
C	-2.462358	4.114293	3.167697
C	-5.780372	3.960450	7.289983
C	6.918830	2.925762	2.575367
C	-4.413951	4.179112	7.327008

C	5.552411	2.707102	2.538342
C	-3.495810	3.234484	6.791220
C	4.634268	3.651730	3.074131
C	-3.924767	2.048678	6.191682
C	5.063225	4.837535	3.673668
C	4.533780	1.849467	6.149356
C	-3.395320	5.036747	3.715994
C	1.347436	0.281667	3.549689
C	-0.208978	6.604548	6.315661
C	0.245028	-0.437961	2.812482
C	0.893430	7.324174	7.052868
C	-4.085958	8.358578	1.616628
C	5.224416	-1.472366	8.248723
C	4.659923	7.756090	0.977350
C	-3.521463	-0.869877	8.888000
C	3.362910	7.859879	1.512886
C	-2.224451	-0.973666	8.352464
C	3.237592	8.563526	2.715447
C	-2.099134	-1.677312	7.149903
C	-2.699825	8.274302	1.039068
C	3.838283	-1.388087	8.826282
C	2.166790	7.260022	0.829977
C	-1.028332	-0.373808	9.035373
C	0.999416	3.087991	9.764427
C	0.139042	3.798223	0.100924
C	-1.210645	2.659023	6.397906
C	2.349104	4.227191	3.467444

O	-2.177350	3.588490	6.905843
O	3.315809	3.297724	2.959507
O	1.273794	-1.219551	5.781621
O	-0.135336	8.105765	4.083730
O	0.745605	4.503123	9.637542
O	0.392853	2.383090	0.227809
S	1.035398	0.220694	5.356750
S	0.103060	6.665519	4.508601

Optimized structure of OMP:

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N	3.7879350	0.8902280	5.5876030
N	-2.5922410	6.1165930	4.1856230
N	2.3342020	2.3866410	6.4684490
N	-1.1385080	4.6201800	3.3047770
N	-0.9737610	-0.2968580	3.3620210
N	2.1694550	7.3036790	6.4112050
H	4.1086300	0.0413220	5.0782560
H	-2.9129360	6.9654990	4.6949700
H	3.4014740	4.7802940	7.6078010
H	-2.2057790	2.2265260	2.1654250
H	-3.9635660	5.2172060	7.6938410
H	5.1592600	1.7896140	2.0793850
H	-3.2124090	1.4226530	5.7446060
H	4.4081030	5.5841680	4.0286200
H	1.3888780	1.3871470	3.2681590
H	-0.1931840	5.6196740	6.5050670
H	2.3486450	-0.1168100	3.3682370
H	-1.1529510	7.1236310	6.4049890
H	6.8579180	-0.8247540	3.1815950
H	-5.6622240	7.8315750	6.5916310
H	2.3489690	-0.2171080	0.9192180
H	-1.1532750	7.2239290	8.8540080
H	-2.6781050	7.8098830	-0.0401660
H	3.8737990	-0.8030620	9.8133920

H -1.9822740 7.7285890 1.5952970

H 3.1779680 -0.7217680 8.1779290

H -1.8900630 5.0066770 9.5578520

H 3.0857570 2.0001440 0.2153740

H 1.2806910 7.6461660 1.1753420

H -0.0849970 -0.6393450 8.5978830

H 2.1877480 6.1629440 0.8359890

H -0.9920540 0.8438770 8.9372370

H 6.0096960 5.4793040 0.4528900

H -4.8140020 1.5275170 9.3203360

H 1.2237390 2.8252670 8.7118570

H -0.0280440 4.1815540 1.0613690

H 4.2613230 5.1547400 0.2623600

H -3.0656290 1.8520810 9.5108660

H -1.2715190 1.7837850 6.8876090

H 2.4672130 5.2230360 2.8856170

H -0.1904370 3.1698630 6.5598390

H 1.3861310 3.8369580 3.2133870

H -1.3062710 2.5837950 5.2844980

H 2.5019660 4.4230250 4.4887270

C 2.4794890 1.2400990 5.8197920

C -1.2837950 5.7667220 3.9534340

C 3.6296670 2.8391080 6.6537930

C -2.4339730 4.1677120 3.1194330

C -5.7438760 4.0845210 7.2502620

C 6.9395710 2.9223000 2.5229640

C -4.3762530 4.2964490 7.2816160

C 5.5719480 2.7103720 2.4916100

C -3.4642220 3.3401710 6.7561570

C 4.6599170 3.6666500 3.0170680

C -3.9006690 2.1490020 6.1728740

C 5.0963630 4.8578190 3.6003510

C 4.5566080 1.9047620 6.1155110

C -3.3609140 5.1020590 3.6577150

C 1.3565210 0.3203420 3.5429430

C -0.1608270 6.6864790 6.2302830

C 0.2487790 -0.4029260 2.8173860

C 0.9469150 7.4097470 6.9558390

C -4.0386690 8.4001200 1.5170780

C 5.2343630 -1.3932990 8.2561480

C 4.7025440 7.7434290 0.8674210

C -3.5068490 -0.7366080 8.9058050

C 3.4072470 7.8609410 1.4042720

C -2.2115530 -0.8541200 8.3689540

C 3.2882000 8.5806910 2.5979060

C -2.0925060 -1.5738700 7.1753190

C -2.6542400 8.3011060 0.9377690

C 3.8499340 -1.2942860 8.8354560

C 2.2065380 7.2586240 0.7316570

C -1.0108440 -0.2518030 9.0415690

C 1.0365580 3.2083960 9.7216400

C 0.1591370 3.7984250 0.0515860

C -1.1829520 2.7476690 6.3655490

C 2.3786470 4.2591520 3.4076770

O -2.1436850 3.6886840 6.8634550

O 3.3393790 3.3181370 2.9097700

O 1.2798220 -1.1515510 5.7942200

O -0.0841280 8.1583720 3.9790060

O 0.7898840 4.6230900 9.5770230

O 0.4058100 2.3837300 0.1962030

S 1.0480550 0.2843290 5.3512860

S 0.1476390 6.7224920 4.4219400