Supporting Information for the Paper:

Synthesis and electronic structure of a two dimensional π-Conjugated Polythiophene.

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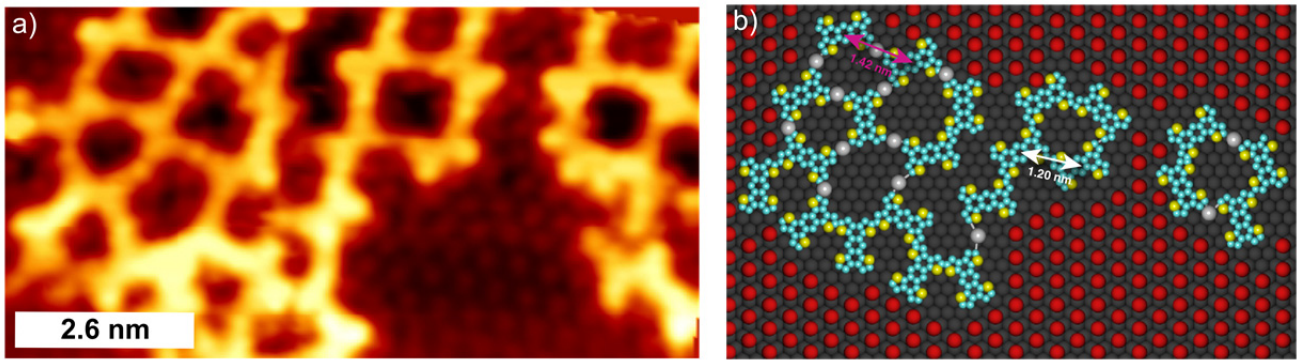


Figure S1: (a) High resolution STM image of polymeric and organometallic structures; coadsorbed atomic Br is observed in a √3×√3 30° reconstruction (U= −0.8 V, I=0.6 nA). (b) Chemical structure as observed in part (a), P^2TTA intermolecular distance of 1.2 nm and organometallic network with TTA–Ag–TTA bonding (1.42 nm).

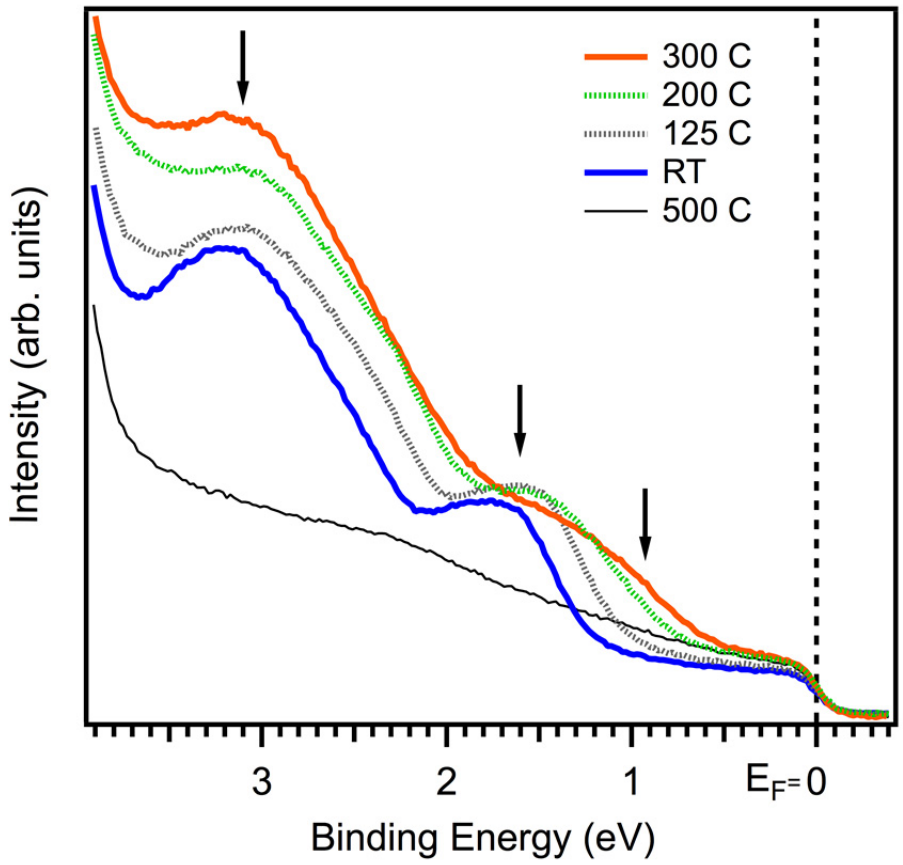


Figure S2: UPS of the valence band region of the molecule(polymer)/Ag(111) interface for different annealing temperatures. A shift of the highest occupied level towards the Fermi level is observed up to 300 °C, after which the electronic states start to vanish due to breaking of the molecule.

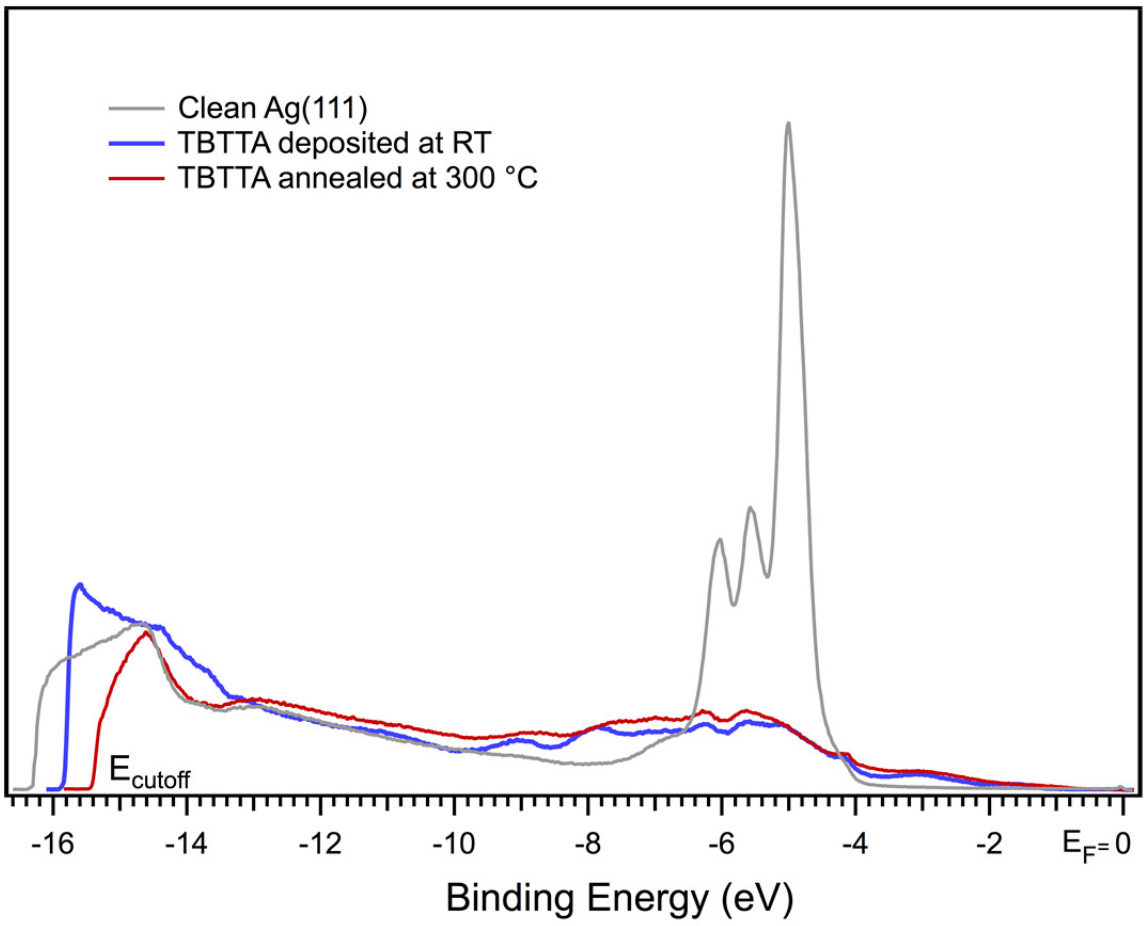


Figure S3: Full valence band region UPS spectra of clean Ag(111) before depositing molecules (gray), after depositing TBTTA (blue) and after annealing-induced polymerization (red).

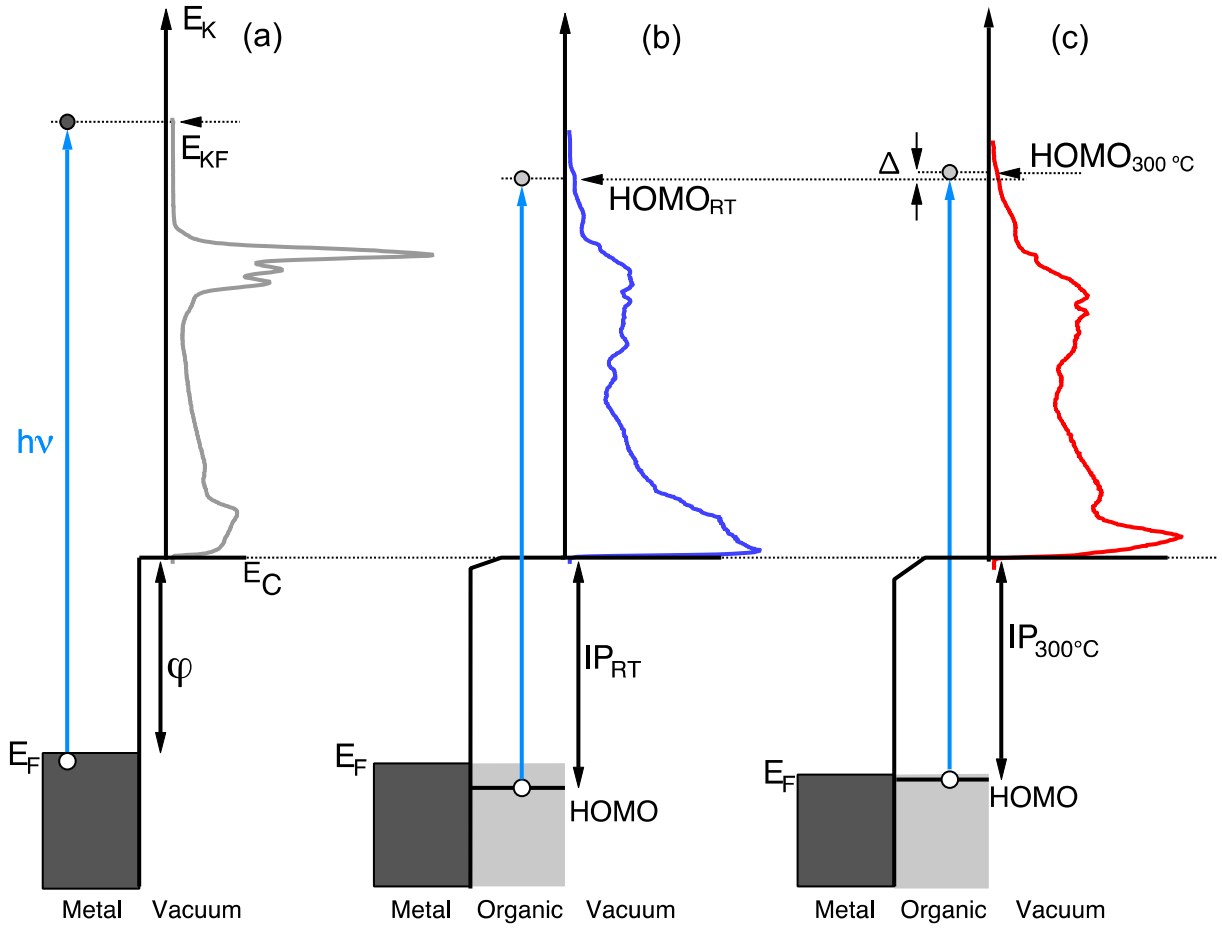


Figure S4: Energy level diagrams in UPS of (a) Ag(111), (b) TBTTA/Ag(111) at room temperature and (c) after annealing.

Figure S3 presents a schematic energy level diagram showing the electronic structure of the clean metal, and of the metal-organic junction before and after annealing. We align the three samples at their vacuum levels, E_C (but Fermi level alignment leads to the same conclusions). The electrons in occupied states at and below the Fermi level E_F are excited by incident photons of energy E=hν, and possess a kinetic energy E_K given by Einstein's photoelectric effect equation ($E_K = h\nu - E_B$, where E_B is the electron binding energy). Electrons that originate from the Fermi level possess the maximum observed kinetic energy E_{KF}, and the average sample work function is given by $\varphi = h\nu - (E_F - E_C)$, [1] where E_C is the minimum kinetic energy observed in the spectrum, arising from the cutoff of the secondary electron tail. Upon deposition of molecules new states appear, which can be directly attributed to the highest occupied molecular orbitals (HOMOs). Annealing produces a shift of the HOMO toward higher energy, given by $\Delta=(HOMO_{300°C} - HOMO_{RT})$, or alternately $\Delta=(IP_{RT} - IP_{300°C})$, where $IP_{300°C}$ and IP_{RT} are the ionization potentials of the annealed and as-deposited samples, respectively. The magnitude of the shift Δ is between 0.2 and 0.6 eV, depending on whether the energy is referenced to the vacuum level or Fermi level, but its sign is positive regardless of the referencing method. We point out that vacuum level referencing is hampered by the surface-averaged nature of the measurement, which convolves local variations in the workfunction across regions of 2D polymer, coadsorbed bromine, and organometallic structures.

[1] N. Koch, J.Phys.: Condens. Matter 20, 184008 (2008)

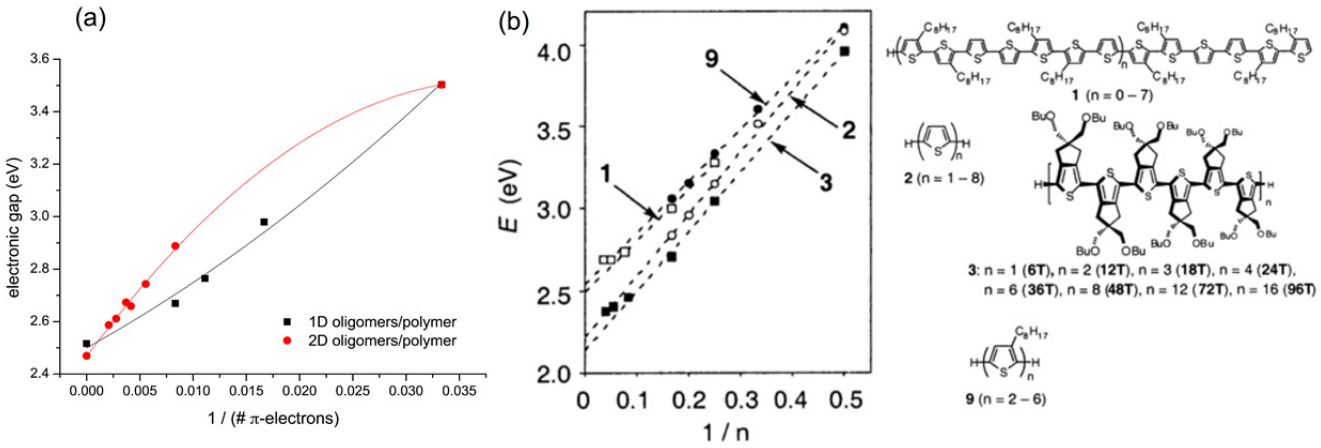


Figure S5: (a) Reduction of the electronic gap in 1D vs. 2D polymer as a function of inverse number of π-electrons. (b) Experimental [2] electronic transition energies (E) as a function of the ring numbers (1/n = 6 × 1/# pi-electrons) of oligothiophenes (shown on the right). The corresponding linear regression are 2.49 + 18.84/#pi-electrons (for series **1**), 2.22 + 22.56/#pi-electrons (for series **2**), 2.13 + 21.84/#pi-electrons (for series **3**). *Adapted from ref. [2]. Copyright 2006 American Chemical Society.*

[2] Izumi, T.; Kobashi, S.; Takimiya, K.; Aso, Y.; Otsubo, T. J. Am. Chem. Soc. 125, 5286 (2003)

Table S1. 2D polymer (**A** and **B**) and 1D polymers (**C**, **D**, **E**, and **F**) that can assemble from TBTTA with corresponding band gap and total energy. Polymer **A** is used for comparison with the experimental structure and its band gap in the main text.

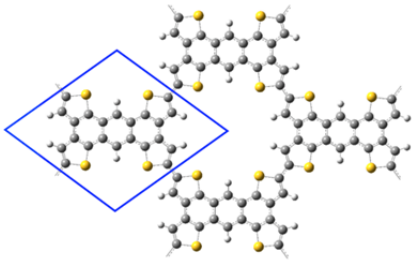
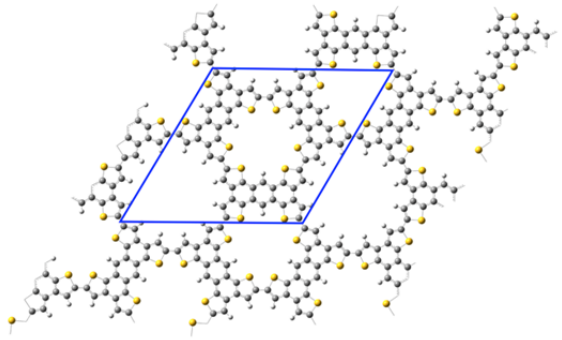
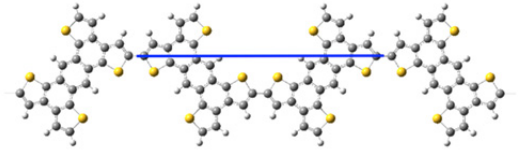
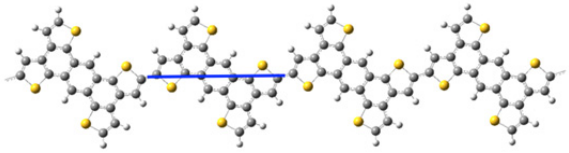
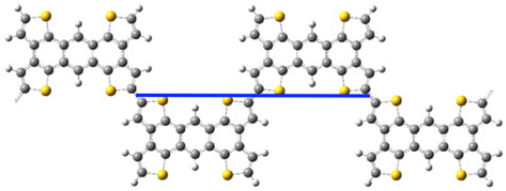
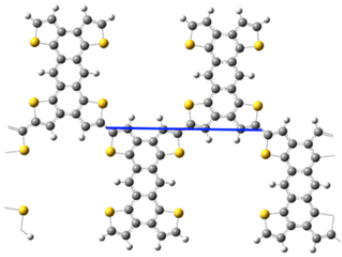
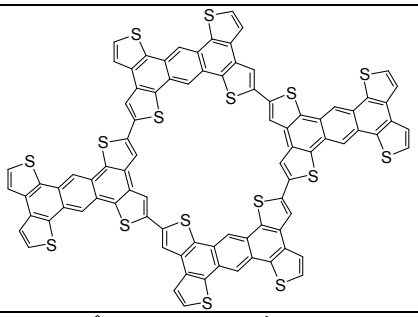
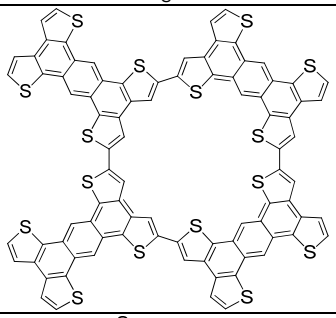
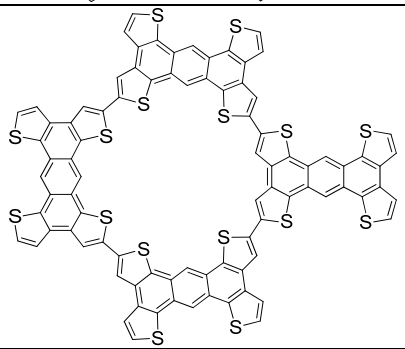
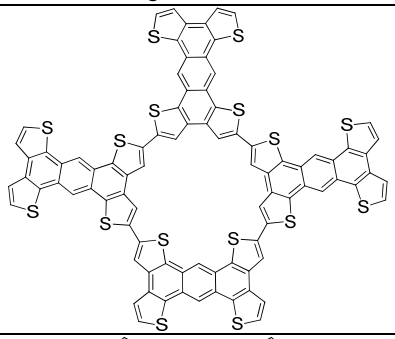
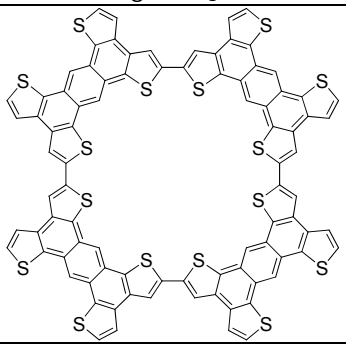
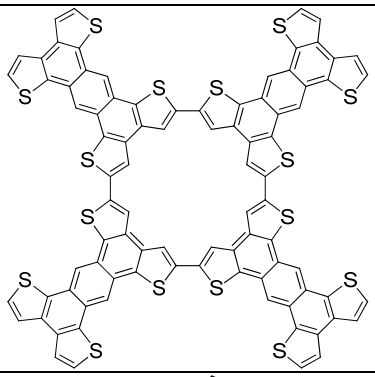
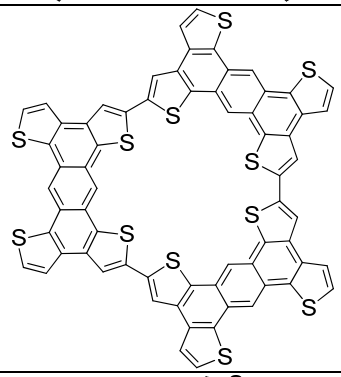
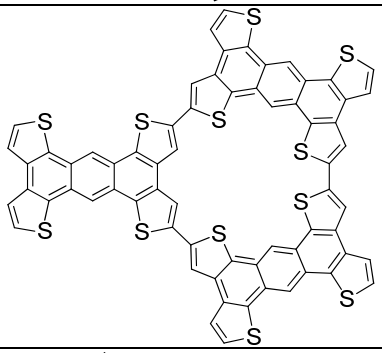
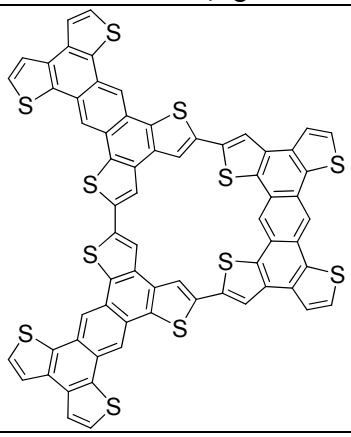
	Polymer structure	HOMO/LUMO band gap (eV)	Total Energy (hartree)
A		2.47	-2434.783328
B		2.48	-7304.302372
C		2.50	-4871.937850
D		2.52	-2435.970962
E		2.85	-4871.941627
F		2.92	-4871.941374

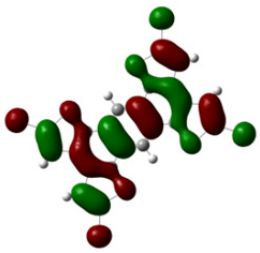
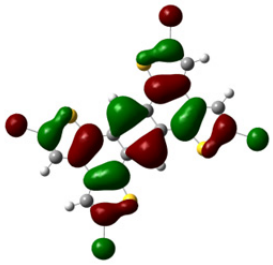
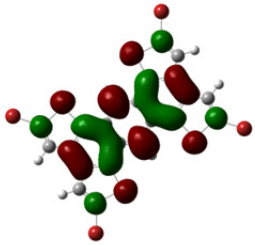
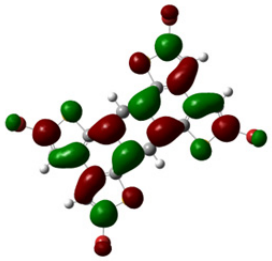
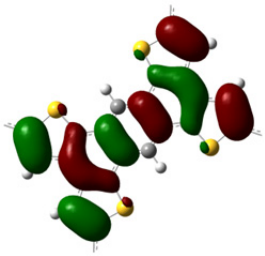
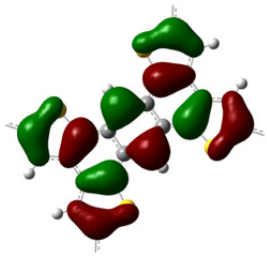
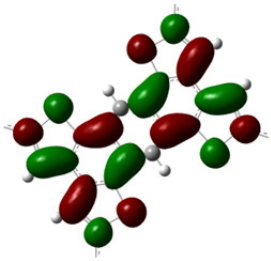
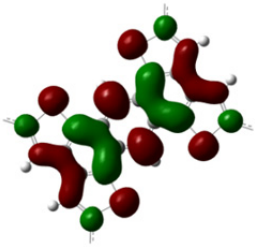
Table S2. Total energy, strain, HOMO energy and HOMO/LUMO gap for cyclic TTA oligomers representing the unit cell of P^2TTA (**1**) and defect clusters (**2-9**).

	Cluster	Total Energy (hartree)	Strain [a)] (eV)	HOMO (eV)	HOMO-LUMO gap (eV)
1		-9743.883354	0.02	-5.08	2.89
2		-9743.878892	0.03	-5.07	2.87
3		-9743.874762	0.14	-5.08	2.87
4		-9743.873786	0.17	-5.10	2.90
5		-9743.857959	0.49	-5.06	2.84

6		-9743.853893	0.60	-5.13	2.94
7		-7307.891752	0.41	-5.08	2.88
8		-7307.866943	1.20	-5.07	2.87
9		-7307.817173	2.55	-5.11	2.91

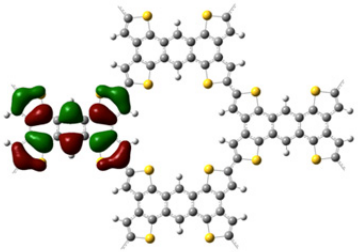
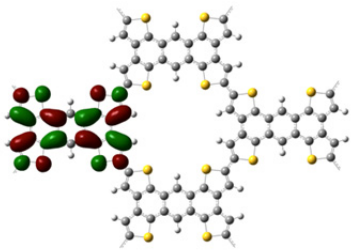
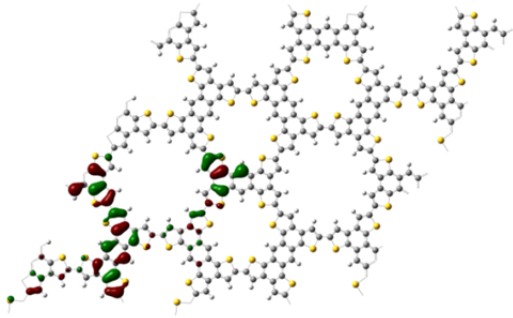
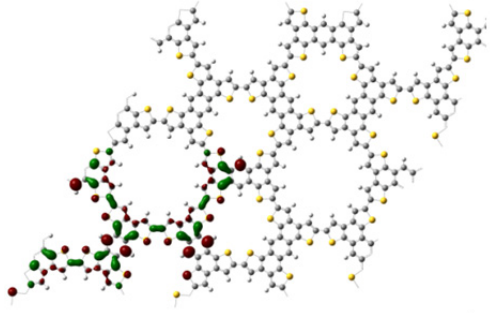
a) Strain energy is calculated as E(cluster)+3*E(monomer H-terminated)-*n**E(cis-dimer)-*m**E(trans-dimer) for the trimer, where *n* is the number of cis-connections in the cluster and *m* the number of trans-connections in the cluster. For tetramers, the formula is E(cluster)+4*E(monomer H-terminated)-*n**E(cis-dimer)-*m**E(trans-dimer).

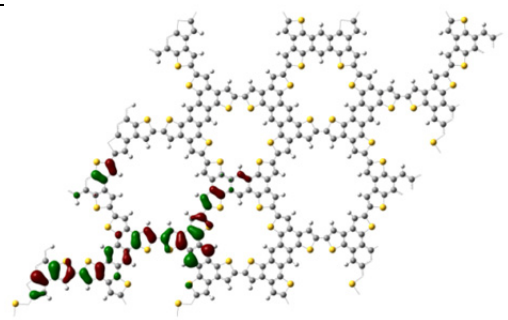
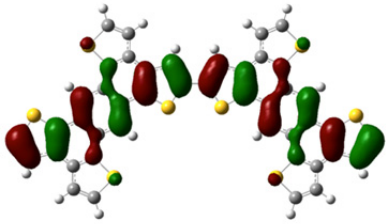
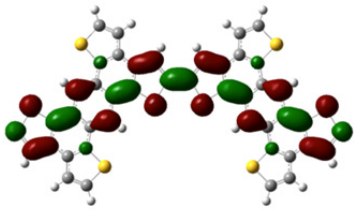
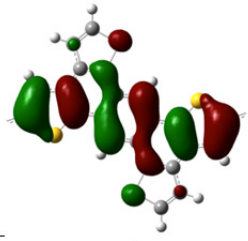
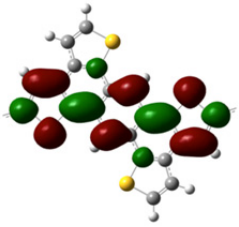
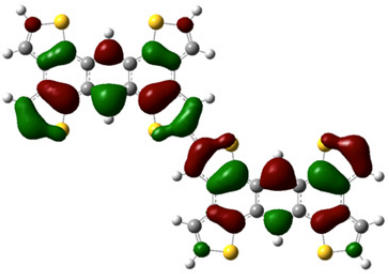
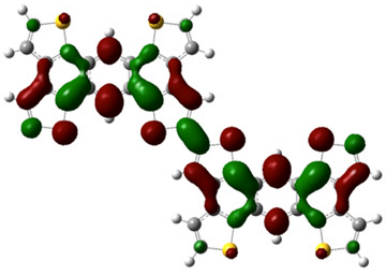
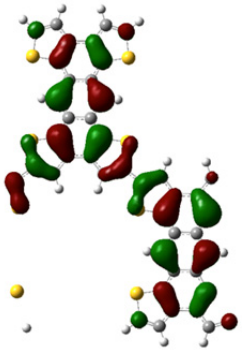
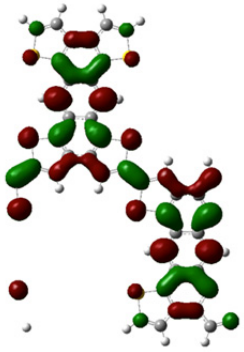
Table S3. Frontier orbitals of **TBTTA** monomer and **P^{2}TTA** polymer (**A**, Table S1).[a)]

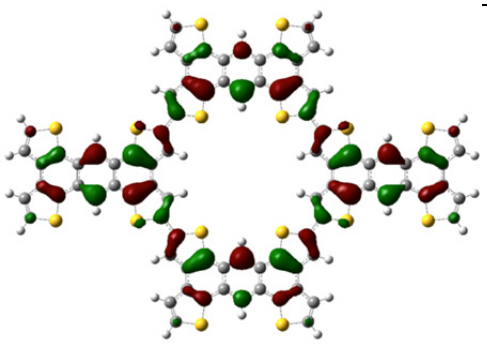
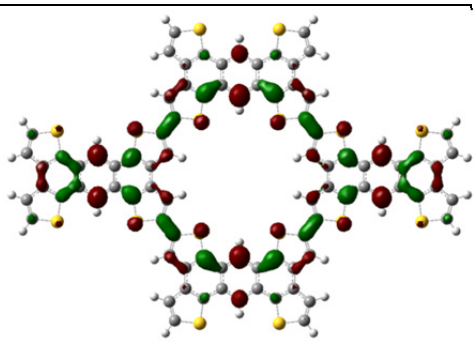
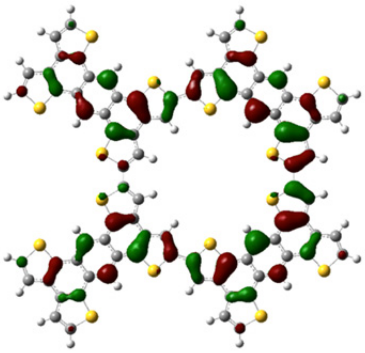
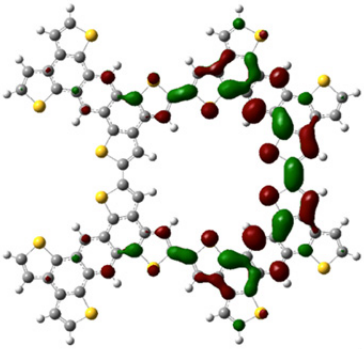
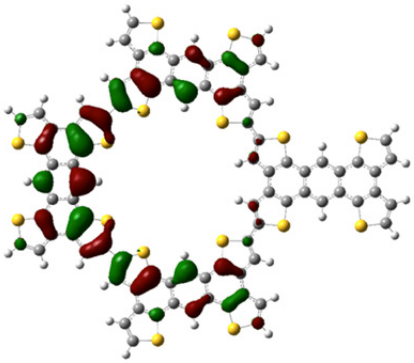
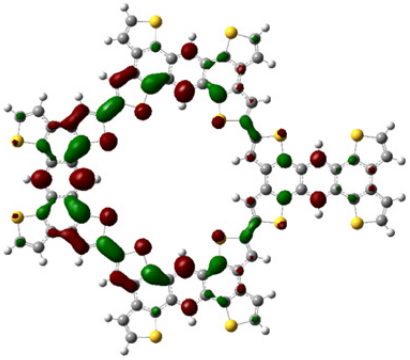
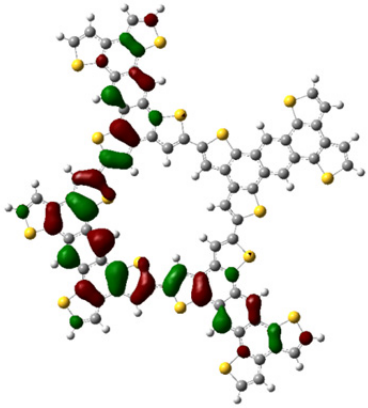
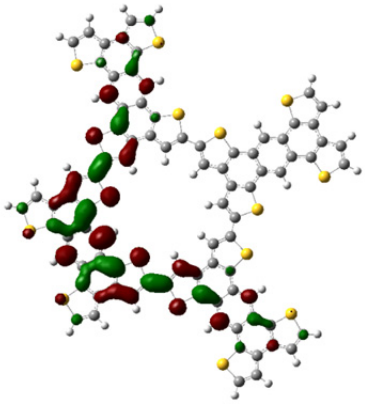
	HOMO-1	HOMO	LUMO	LUMO+1
TBTTA				
P^{2}TTA (A)				

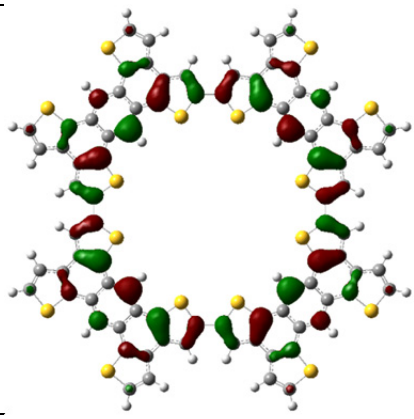
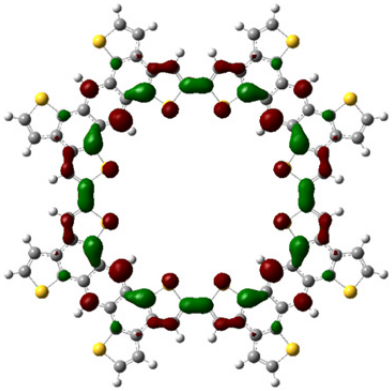
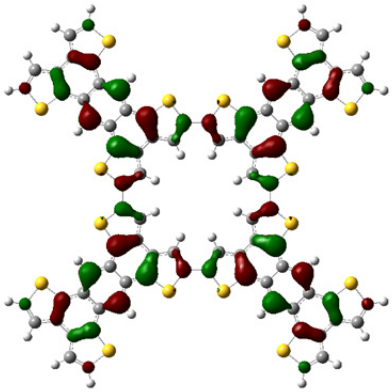
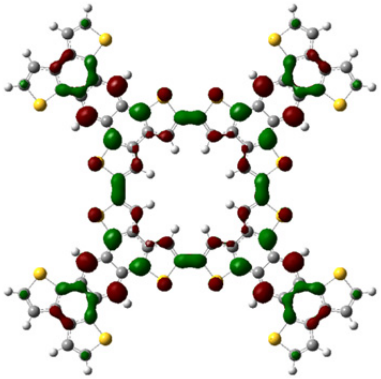
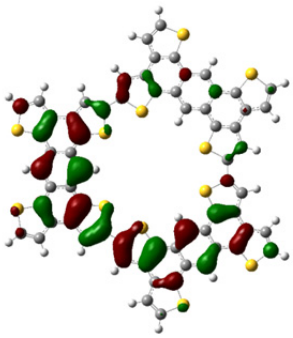
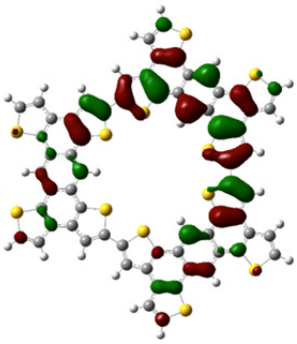
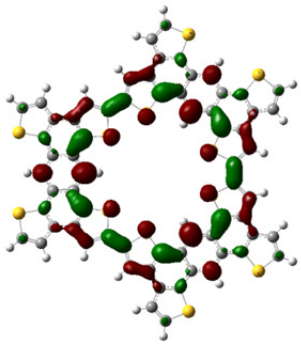
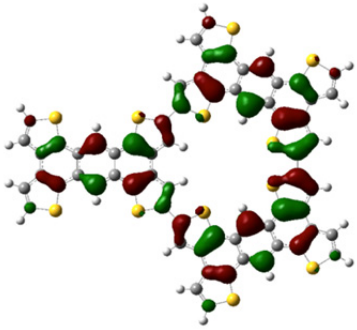
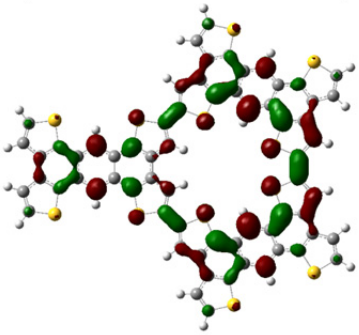
a) While the HOMO and the HOMO-1 orbital topology is the same for the monomer and the polymer, the order is reversed for the unoccupied states (the LUMO of the polymer has topography of the LUMO+1 of the monomer and the LUMO+1 of the monomer has the topography of the LUMO of the polymer).

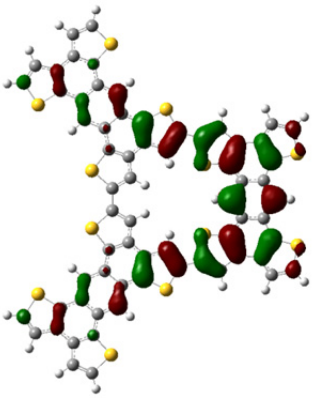
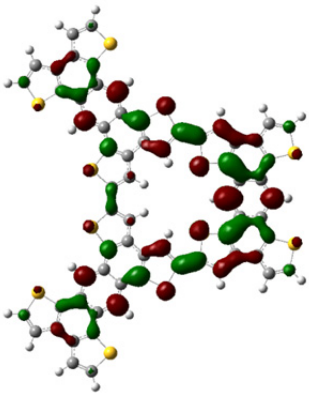
Table S4. Frontier orbitals of **TTA** polymers (2D polymers **A, B**; 1D polymers **C-F**) and cyclic oligomers (**1-9**) from Tables S1 and S2.

	HOMO	LUMO
A		
B		

degenerate HOMO of **B**		
C		
D		
E		
F		

1		
2		
3		
4		

5		
6		
7	 and 	
8		

9		

X Y Z coordinates (in Angstroms) of DFT-optimized (B3LYP/6-31G*) molecular/polymer structures

For PBC calculations, the 2D translation vectors (Tv) appear at the end of the list of coordinates.

Table S1, Structure A

C	-2.60546119	-2.74908201	0.00006473
C	-3.44311404	-1.57817390	0.00005943
C	-2.83798906	-0.31914900	0.00004225
C	-1.41740646	-0.12564707	0.00002244
C	-0.57672864	-1.30078592	0.00002183
C	-1.21849217	-2.58276578	0.00004725
C	0.81228591	-1.13551593	-0.00000045
C	1.41740646	0.12564707	-0.00002224
C	0.57672864	1.30078592	-0.00001857
C	1.21849218	2.58276578	-0.00004016
C	2.60546119	2.74908202	-0.00006137
C	3.44311404	1.57817390	-0.00006472
C	2.83798905	0.31914900	-0.00004834
C	-0.81228591	1.13551593	0.00000220
C	4.86668540	1.50632390	-0.00005602
C	5.35638221	0.22159318	-0.00002676
C	2.99686833	4.11968352	-0.00004787
C	1.93895185	4.99775865	-0.00001810
C	-2.99686833	-4.11968353	0.00005724
C	-1.93895184	-4.99775865	0.00002677
C	-4.86668540	-1.50632390	0.00004398
C	-5.35638226	-0.22159318	0.00001679
S	-4.04063580	0.95344539	0.00004494
S	-0.40217698	-4.13172580	0.00006822
S	4.04063580	-0.95344539	-0.00005869
S	0.40217698	4.13172580	-0.00005343
H	1.44487159	-2.01961935	-0.00000157
H	-1.44487159	2.01961935	0.00000263
H	5.51039567	2.37922944	-0.00004693
H	4.03063351	4.44779282	-0.00004333
H	-4.03063351	-4.44779282	0.00004954
H	-5.51039567	-2.37922944	0.00003641
Tv	12.08851108	0.00000000	0.00000000
Tv	3.90227316	11.44075814	0.00000000

Table S1, Structure B

C	-12.46453216	-3.69308243	0.00000000
C	-13.63749598	-5.84019341	0.00000000
C	-12.45579873	-6.59420266	0.00000000
C	-11.19910481	-5.86878577	0.00000000
C	-11.26104290	-4.46843123	0.00000000
C	-9.84523342	-6.34714158	0.00000000
C	-8.90000888	-5.34109552	0.00000000
C	-12.71862706	-8.00582264	0.00000000
C	-14.06255535	-8.32102802	0.00000000
S	-9.68037020	-3.76046099	0.00000000
H	-11.54669752	-1.75078063	0.00000000
H	-9.58300364	-7.39969759	0.00000000
H	-11.93843862	-8.75943239	0.00000000
S	-16.54919179	-9.46689294	0.00000000
C	-5.14573961	-5.86874418	0.00000000
C	-3.88902184	-6.59419532	0.00000000
C	-2.70735836	-5.84009549	0.00000000
C	-2.63794082	-4.41026785	0.00000000
C	-3.88032720	-3.69302852	0.00000000
C	-5.08382160	-4.46838378	0.00000000

C	-3.85706114	-2.29429982	0.00000000
C	-2.65735503	-1.57465716	0.00000000
C	-1.41495966	-2.29190550	0.00000000
C	-0.21144630	-1.51658127	0.00000000
C	-0.14952129	-0.11621687	0.00000000
C	-1.40622710	0.60920125	0.00000000
C	-2.58791447	-0.14481455	0.00000000
C	-1.43823172	-3.69063219	0.00000000
C	-1.66906212	2.02081822	0.00000000
C	-3.01300868	2.33602829	0.00000000
C	1.20432720	0.36214800	0.00000000
C	2.14952392	-0.64392528	0.00000000
C	-6.49960209	-6.34711104	0.00000000
C	-7.44485285	-5.34107269	0.00000000
C	-3.62608669	-8.00571040	0.00000000
C	-2.28208918	-8.32096153	0.00000000
S	-1.30384425	-6.85463484	0.00000000
S	-6.66450611	-3.76043902	0.00000000
S	-3.99139744	0.86985077	0.00000000
S	1.36922716	-2.22456701	0.00000000
H	-4.79826501	-1.75088553	0.00000000
H	-0.49702786	-4.23404948	0.00000000
H	-0.88885852	2.77440948	0.00000000
H	1.46656877	1.41470143	0.00000000
H	-6.76183467	-7.39966747	0.00000000
H	-4.40616545	-8.75943681	0.00000000
C	7.16039674	0.60915877	0.00000000
C	5.90370281	-0.11626812	0.00000000
C	5.96562088	-1.51663564	0.00000000
C	7.16912516	-2.29196845	0.00000000
C	8.41151349	-1.57472581	0.00000000
C	8.34208198	-0.14485646	0.00000000
C	9.61124807	-2.29432816	0.00000000
C	8.39214969	-4.41032106	0.00000000
C	7.19242612	-3.69070872	0.00000000
C	7.42320109	2.02079278	0.00000000
C	8.76714439	2.33601315	0.00000000
C	4.54985945	0.36210766	0.00000000
C	3.60465589	-0.64395043	0.00000000
S	4.38493719	-2.22460486	0.00000000
S	9.74552900	0.86985766	0.00000000
S	7.05809622	-6.85486948	0.00000000
H	6.25123468	-4.23413519	0.00000000
H	6.64301063	2.77439254	0.00000000
H	4.28760666	1.41465970	0.00000000
C	-6.94958674	5.85931964	0.00000000
C	-5.67652204	5.20463140	0.00000000
C	-4.43280364	5.85110244	0.00000000
C	-4.43289826	7.30217154	0.00000000
C	-5.67660659	7.94862738	0.00000000
C	-8.17253449	5.18010724	0.00000000
C	-3.34183978	8.23553867	0.00000000
C	-3.74074142	9.55711101	0.00000000
C	-3.34173262	4.91774126	0.00000000
C	-3.74057455	3.59614872	0.00000000
S	-5.49965366	3.48188496	0.00000000
H	-8.17257699	4.09332955	0.00000000
H	-2.29915263	7.93637263	0.00000000
H	-2.29904434	5.21690463	0.00000000
C	10.18677179	7.30218102	0.00000000
C	10.18683243	5.85113195	0.00000000
C	11.43060683	5.20473904	0.00000000
C	12.70363681	5.85937273	0.00000000
C	12.70351591	7.29398786	0.00000000
C	11.43057800	7.94849395	0.00000000
C	13.92653759	7.97313617	0.00000000

C	15.14940149	7.29390074	0.00000000
C	9.09583198	8.23572404	0.00000000
C	9.49487684	9.55725834	0.00000000
C	9.09578690	4.91772581	0.00000000
C	9.49472753	3.59614942	0.00000000
S	11.25375487	3.48190609	0.00000000
H	13.92663410	9.05992180	0.00000000
H	8.05306305	7.93686576	0.00000000
H	8.05309872	5.21685985	0.00000000
S	11.25380734	9.67186128	0.00000000
Tv	22.09908217	0.00000000	0.00000000
Tv	11.04936707	19.13827134	0.00000000

Table S1, Structure C

C	4.08517491	3.38494150	-0.00002642
C	2.94699843	2.50374977	-0.00000340
C	3.16600477	1.12330098	0.00002809
C	4.47098046	0.53011302	0.00003896
C	5.61261552	1.41364532	0.00001497
C	5.36525378	2.82936887	-0.00001684
C	6.89445662	0.85688551	0.00002358
C	7.11192059	-0.52612587	0.00006005
C	5.97022757	-1.40969723	0.00009503
C	6.21761923	-2.82533875	0.00015284
C	7.49768940	-3.38120239	0.00017643
C	8.63579063	-2.49977473	0.00014040
C	8.41687637	-1.11939985	0.00008091
C	4.68845449	-0.85294735	0.00007843
C	10.01946624	-2.83889837	0.00014117
C	10.85859017	-1.74796806	0.00004774
C	7.47662549	-4.81484888	0.00024118
C	6.21282070	-5.32264003	0.00028777
C	4.10633064	4.81876609	-0.00004517
C	5.36993728	5.32669003	-0.00003877
C	1.56340983	2.84286849	-0.00000517
C	0.72424391	1.75192914	0.00000026
S	1.64869754	0.25136511	0.00005879
S	6.58911933	4.08273021	-0.00005788
S	9.93421957	-0.24744094	0.00008021
S	4.99391390	-4.07891492	0.00019889
H	7.75427859	1.52227295	0.00000938
H	3.82857044	-1.51826085	0.00010462
H	10.38438944	-3.85954542	0.00017132
H	8.36641421	-5.43445021	0.00026731
H	3.21628923	5.43806616	-0.00004831
H	1.19836566	3.86347842	-0.00003332
C	-8.63571154	-2.49979985	-0.00012843
C	-7.49755360	-3.38118007	-0.00017446
C	-6.21750943	-2.82529815	-0.00015987
C	-5.97014383	-1.40965118	-0.00010105
C	-7.11185701	-0.52609763	-0.00005605
C	-8.41677859	-1.11939824	-0.00006893
C	-6.89441276	0.85691845	-0.00001457
C	-5.61257349	1.41368423	-0.00001095
C	-4.47092136	0.53016661	-0.00004595
C	-3.16597567	1.12336624	-0.00004107
C	-2.94693179	2.50383796	-0.00000857
C	-4.08516149	3.38499012	0.00002546
C	-5.36522198	2.82941317	0.00002287
C	-4.68837556	-0.85289548	-0.00008943
C	-4.10632079	4.81881805	0.00005023
C	-5.36992649	5.32674065	0.00005283
C	-1.56338394	2.84297256	-0.00001080

C	-0.72426388	1.75194570	-0.00001724
C	-10.01933936	-2.83896152	-0.00012320
C	-10.85843440	-1.74795764	-0.00003076
C	-7.47647549	-4.81482909	-0.00024423
C	-6.21266394	-5.32260548	-0.00030283
S	-4.99377948	-4.07885228	-0.00021493
S	-9.93417890	-0.24753828	-0.00004221
S	-6.58909972	4.08276416	0.00007393
S	-1.64862935	0.25150323	-0.00009379
H	-7.75424169	1.52229671	0.00000964
H	-3.82848470	-1.51819968	-0.00012364
H	-3.21625722	5.43808866	0.00005038
H	-1.19824467	3.86353382	0.00002037
H	-10.38434059	-3.85956664	-0.00015437
H	-8.36627774	-5.43440943	-0.00026738
H	-5.66942014	6.36627121	0.00006043
H	5.66941494	6.36622556	-0.00004035
H	5.91275289	-6.36202916	0.00034935
H	-5.91257044	-6.36198642	-0.00037042
Tv	23.16551133	0.00000000	0.00000000

Table S1, Structure D

C	-3.44198400	1.57908200	0.00000000
C	-2.60573900	2.75017300	0.00000000
C	-1.21972500	2.58591200	0.00000000
C	-0.57659800	1.30103900	0.00000000
C	-1.41649400	0.12665200	0.00000000
C	-2.83696400	0.31980200	0.00000000
C	-0.81109800	-1.13564600	0.00000000
C	0.57659800	-1.30103900	0.00000000
C	1.41649400	-0.12665200	0.00000000
C	2.83696400	-0.31980200	0.00000000
C	3.44198400	-1.57908200	0.00000000
C	2.60573900	-2.75017300	0.00000000
C	1.21972500	-2.58591200	0.00000000
C	0.81109800	1.13564600	0.00000000
C	2.99821300	-4.12926100	0.00000000
C	1.93402300	-4.97904700	0.00000000
C	4.86598000	-1.50623000	0.00000000
C	5.35599000	-0.22176000	0.00000000
C	-4.86598000	1.50623000	0.00000000
C	-5.35599000	0.22176000	0.00000000
C	-2.99821300	4.12926100	0.00000000
C	-1.93402300	4.97904700	0.00000000
S	-0.40836900	4.13865200	0.00000000
S	-4.03994300	-0.95347400	0.00000000
S	0.40836900	-4.13865200	0.00000000
S	4.03994300	0.95347400	0.00000000
H	-1.44374500	-2.01979000	0.00000000
H	1.44374500	2.01979000	0.00000000
H	4.02869200	-4.46653000	0.00000000
H	5.50961400	-2.37922000	0.00000000
H	-5.50961400	2.37922000	0.00000000
H	-4.02869200	4.46653000	0.00000000
H	1.94615100	-6.06080000	0.00000000
H	-1.94615100	6.06080000	0.00000000
Tv	12.08764200	0.00000000	0.00000000

Table S1, Structure E

C	-1.20039229	2.79654579	0.00000584

C	-1.19989444	4.23556407	0.00000684
C	-2.42325719	4.90780364	0.00000466
C	-3.69302539	4.23657673	0.00000344
C	-3.69281047	2.79272774	0.00000544
C	-2.42430556	2.12374715	0.00000666
C	-4.91876521	2.11853739	0.00000625
C	-6.14473858	2.79276723	0.00000107
C	-6.14454441	4.23656396	-0.00000393
C	-7.41431745	4.90782026	-0.00001216
C	-8.63764563	4.23552468	-0.00001634
C	-8.63711464	2.79659427	-0.00000934
C	-7.41325079	2.12374861	0.00000084
C	-4.91876060	4.90961900	-0.00000175
C	-9.75377536	1.90937604	-0.00001142
C	-9.40607401	0.57959525	-0.00000208
C	-9.75871857	5.12933837	-0.00002642
C	-9.38680216	6.43952791	-0.00003006
C	-0.08378739	1.90935900	0.00000492
C	-0.43161520	0.57958718	0.00000358
C	-0.07888168	5.12937421	0.00000693
C	-0.45088655	6.43959384	0.00000657
S	-2.18046766	6.64293539	0.00000390
S	-2.18575121	0.38856348	0.00000589
S	-7.65177018	0.38854461	0.00000961
S	-7.65708366	6.64292328	-0.00002139
H	-4.91880795	1.03134352	0.00000825
H	-4.91876781	5.99678178	-0.00000475
H	-10.78501830	2.24542294	-0.00001941
H	-10.79315719	4.80438738	-0.00003142
H	0.94747221	2.24533224	0.00000292
H	0.95557191	4.80453217	0.00000893
C	8.63633918	-4.23693206	0.00001534
C	8.63578109	-2.79794570	0.00000534
C	7.41188331	-2.12514009	-0.00000784
C	6.14336904	-2.79411972	-0.00000907
C	6.14319190	-4.23793842	-0.00000107
C	7.41295288	-4.90916274	0.00001016
C	4.91743413	-4.91101541	-0.00000226
C	3.69169190	-4.23796116	-0.00000544
C	3.69145301	-2.79412821	-0.00000944
C	2.42293315	-2.12517664	-0.00000666
C	1.19903295	-2.79801126	-0.00000384
C	1.19857303	-4.23699147	-0.00000185
C	2.42193277	-4.90922805	-0.00000267
C	4.91740069	-2.11990187	-0.00001325
C	0.07747022	-5.13077178	0.00000107
C	0.44955506	-6.44097926	0.00000243
C	0.08239709	-1.91084852	-0.00000092
C	0.43019390	-0.58107576	-0.00000059
C	9.75737110	-5.13073282	0.00003342
C	9.38528973	-6.44093965	0.00004206
C	9.75239085	-1.91074956	0.00000842
C	9.40476347	-0.58094963	-0.00000192
S	7.65040671	-0.38993509	-0.00001661
S	7.65569311	-6.64427080	0.00002739
S	2.17915622	-6.64435077	0.00000110
S	2.18433380	-0.38999506	-0.00000589
H	4.91743334	-5.99817721	0.00000374
H	4.91743243	-1.03271002	-0.00001625
H	-0.95694552	-4.80584966	0.00000107
H	-0.94884844	-2.24685774	0.00000208
H	10.79183395	-4.80590878	0.00004042
H	10.78364278	-2.24678944	0.00001941
H	-10.02554381	7.31268844	-0.00003868
H	-0.18905624	-7.31422637	0.00000481
H	10.02391549	-7.31416340	0.00005567

H	0.18776382	7.31280302	0.00000719
Tv	19.67263844	0.00000000	0.00000000

Table S1, Structure F

C	-3.41654233	1.19323177	-0.03068544
C	-1.97676902	1.19331507	-0.03089763
C	-1.30525603	2.41757781	-0.05925615
C	-1.97461245	3.68547883	-0.08779744
C	-3.41878714	3.68538146	-0.08773949
C	-4.08807909	2.41747389	-0.05898730
C	-4.09228486	4.91122413	-0.11524702
C	-3.41841629	6.13640802	-0.14278294
C	-1.97499548	6.13649321	-0.14270676
C	-1.30412882	7.40616644	-0.17136623
C	-1.97748941	8.62871289	-0.19953177
C	-3.41583493	8.62864964	-0.19970682
C	-4.08926927	7.40612411	-0.17165098
C	-1.30112320	4.91129968	-0.11523230
C	-4.30979883	9.74967504	-0.22603451
C	-5.62015207	9.37872997	-0.21798593
C	-1.08340239	9.74969080	-0.22556221
C	0.22692776	9.37857975	-0.21716975
C	-4.30393375	0.07747464	-0.00453016
C	-5.63350724	0.42684116	-0.01242429
C	-1.08939028	0.07756804	-0.00505283
C	0.24016074	0.42687925	-0.01323866
S	0.42968358	2.18045189	-0.05432648
S	-5.82291882	2.18047661	-0.05357332
S	-5.82465686	7.64954962	-0.17783258
S	0.43118406	7.64934916	-0.17703029
H	-5.17946127	4.91182487	-0.11513312
H	-0.21394517	4.91165309	-0.11519220
H	-3.98407814	10.78360887	-0.24991563
H	-1.40897268	10.78369103	-0.24948196
H	-3.96902803	-0.95387351	0.01957300
H	-1.42423816	-0.95376282	0.01898285
H	-6.49277340	10.01802816	-0.23311860
H	1.09963978	10.01776772	-0.23202887
C	3.61901586	-8.63551700	0.18547609
C	5.05735979	-8.63553079	0.18659614
C	5.73089362	-7.41301765	0.16018328
C	5.06014451	-6.14322187	0.13211022
C	3.61672458	-6.14324705	0.13114504
C	2.94575829	-7.41290087	0.15809553
C	2.94293647	-4.91799214	0.10455156
C	3.61649606	-3.69217516	0.07872870
C	5.06068072	-3.69212964	0.07944875
C	5.73001382	-2.42421540	0.05216154
C	5.05847593	-1.19995130	0.02514768
C	3.61870433	-1.19996057	0.02481688
C	2.94714635	-2.42424603	0.05114640
C	5.73409153	-4.91804872	0.10617529
C	2.73135873	-0.08414999	-0.00012593
C	1.40180333	-0.43345527	0.00644590
C	5.94583528	-0.08411568	0.00015841
C	2.72483597	-9.75646040	0.20974754
C	1.41453716	-9.38525183	0.20077708
C	5.95123283	-9.75663366	0.21237484
C	7.26161754	-9.38576610	0.20553526
S	1.21042526	-7.65596591	0.16229359
S	1.21221818	-2.18710192	0.04466074
H	1.85575914	-4.91827053	0.10400047
H	6.82126986	-4.91869844	0.10678339

H	3.06622227	0.94722312	-0.02215862
H	5.61089049	0.94724883	-0.02274174
H	3.05031686	-10.79050607	0.23287231
H	5.62542092	-10.79056696	0.23505698
H	0.54177113	-10.02439167	0.21435420
C	-6.79519221	-0.43344934	0.00742354
S	-6.60435792	-7.65657094	0.16717088
S	-6.60567108	-2.18713902	0.04660756
H	-5.93638675	-10.02510982	0.22059894
Tv	14.07059234	0.00000000	0.00000000

Table S2, Structure 1

C	3.71832000	-6.31488200	0.00000000
C	3.71899600	-7.75388200	0.00000000
C	2.49576200	-8.42636800	0.00000000
C	1.22579800	-7.75539500	0.00000000
C	1.22591400	-6.31161200	0.00000000
C	2.49423300	-5.64229600	0.00000000
C	0.00005700	-5.63734600	0.00000000
C	-1.22585100	-6.31153200	0.00000000
C	-1.22580500	-7.75532500	0.00000000
C	-2.49581400	-8.42621300	0.00000000
C	-3.71900900	-7.75366200	0.00000000
C	-3.71829900	-6.31464100	0.00000000
C	-2.49413700	-5.64217400	0.00000000
C	-0.00002600	-8.42845400	0.00000000
C	-4.83448700	-5.42699000	0.00000000
C	-4.48573500	-4.09738100	0.00000000
C	-4.84034200	-8.64713900	0.00000000
C	-4.46878700	-9.95742600	0.00000000
C	4.83458000	-5.42724000	0.00000000
C	4.48589700	-4.09768100	0.00000000
C	4.84028700	-8.64741700	0.00000000
C	4.46867600	-9.95768600	0.00000000
S	2.73895700	-10.16147000	0.00000000
S	2.73185600	-3.90717400	0.00000000
S	-2.73173500	-3.90704500	0.00000000
S	-2.73908300	-10.16130100	0.00000000
H	0.00009700	-4.55016000	0.00000000
H	-0.00005100	-9.51561400	0.00000000
H	-5.86593900	-5.76241600	0.00000000
H	-5.87470600	-8.32194500	0.00000000
H	5.86600800	-5.76275400	0.00000000
H	5.87467100	-8.32228700	0.00000000
C	-6.11458700	0.72000200	0.00000000
C	-6.11453400	-0.71967300	0.00000000
C	-7.33898000	-1.39130000	0.00000000
C	-8.60720700	-0.72203600	0.00000000
C	-8.60725200	0.72225900	0.00000000
C	-7.33904500	1.39157300	0.00000000
C	-9.83346700	1.39561000	0.00000000
C	-11.05901700	0.72175800	0.00000000
C	-11.05897500	-0.72167000	0.00000000
C	-12.32892900	-1.39256200	0.00000000
C	-13.55182700	-0.71921500	0.00000000
C	-13.55186800	0.71916300	0.00000000
C	-12.32900800	1.39258000	0.00000000
C	-9.83339100	-1.39545700	0.00000000
C	-14.67323200	1.61317700	0.00000000
C	-14.30232700	2.92356800	0.00000000
C	-14.67314100	-1.61329100	0.00000000
C	-14.30215900	-2.92366100	0.00000000
C	-4.99824000	1.60697900	0.00000000

C	-5.34704600	2.93661300	0.00000000
C	-4.99815100	-1.60659200	0.00000000
C	-5.34691100	-2.93624500	0.00000000
S	-7.10109400	-3.12630000	0.00000000
S	-7.10128300	3.12659100	0.00000000
S	-12.57257500	3.12797400	0.00000000
S	-12.57239800	-3.12797000	0.00000000
H	-9.83400900	2.48279200	0.00000000
H	-9.83387600	-2.48263900	0.00000000
H	-15.70746200	1.28750100	0.00000000
H	-15.70739000	-1.28767200	0.00000000
H	-3.96674400	1.27176000	0.00000000
H	-3.96667100	-1.27133600	0.00000000
C	3.71893800	7.75375500	0.00000000
C	3.71823600	6.31472800	0.00000000
C	2.49405800	5.64229200	0.00000000
C	1.22579800	6.31169400	0.00000000
C	1.22573600	7.75550200	0.00000000
C	2.49577100	8.42634200	0.00000000
C	-0.00002500	8.42861300	0.00000000
C	-1.22586700	7.75554600	0.00000000
C	-1.22598700	6.31177800	0.00000000
C	-2.49430300	5.64248700	0.00000000
C	-3.71843100	6.31500800	0.00000000
C	-3.71907300	7.75401700	0.00000000
C	-2.49582300	8.42650800	0.00000000
C	-0.00011100	5.63751000	0.00000000
C	-4.84034200	8.64757500	0.00000000
C	-4.46872500	9.95784200	0.00000000
C	-4.83465700	5.42738600	0.00000000
C	-4.48593500	4.09777400	0.00000000
C	4.84031000	8.64718700	0.00000000
C	4.46879200	9.95748200	0.00000000
C	4.83444000	5.42708200	0.00000000
C	4.48568600	4.09745600	0.00000000
S	2.73170900	3.90715400	0.00000000
S	2.73908700	10.16143200	0.00000000
S	-2.73900900	10.16160800	0.00000000
S	-2.73191800	3.90737100	0.00000000
H	-0.00001000	9.51577500	0.00000000
H	-0.00016500	4.55032800	0.00000000
H	-5.87473100	8.32245700	0.00000000
H	-5.86610000	5.76284400	0.00000000
H	5.87465500	8.32193700	0.00000000
H	5.86588600	5.76251800	0.00000000
C	13.55192600	0.71892600	0.00000000
C	13.55190700	-0.71944500	0.00000000
C	12.32901400	-1.39281400	0.00000000
C	11.05906000	-0.72193800	0.00000000
C	11.05907400	0.72148100	0.00000000
C	12.32905500	1.39232700	0.00000000
C	9.83351800	1.39532600	0.00000000
C	8.60726800	0.72197500	0.00000000
C	8.60728200	-0.72232700	0.00000000
C	7.33904100	-1.39156300	0.00000000
C	6.11469900	-0.71997700	0.00000000
C	6.11461200	0.71970000	0.00000000
C	7.33907800	1.39131700	0.00000000
C	9.83346500	-1.39573600	0.00000000
C	4.99820800	1.60664600	0.00000000
C	5.34696500	2.93629000	0.00000000
C	4.99829600	-1.60695400	0.00000000
C	5.34701700	-2.93656100	0.00000000
C	14.67328300	1.61295400	0.00000000
C	14.30235700	2.92333800	0.00000000
C	14.67323600	-1.61350600	0.00000000

C	14.30228600	-2.92388100	0.00000000
S	12.57252200	-3.12821700	0.00000000
S	12.57260300	3.12772200	0.00000000
S	7.10112900	3.12631300	0.00000000
S	7.10119000	-3.12665900	0.00000000
H	9.83407000	2.48250500	0.00000000
H	9.83397900	-2.48291300	0.00000000
H	3.96671700	1.27141900	0.00000000
H	3.96692100	-1.27141400	0.00000000
H	15.70751800	1.28729100	0.00000000
H	15.70748000	-1.28786900	0.00000000
H	-14.94163600	3.79633800	0.00000000
H	-14.94142100	-3.79646500	0.00000000
H	-5.10782800	-10.83037000	0.00000000
H	5.10767900	-10.83065800	0.00000000
H	-5.10771500	10.83082400	0.00000000
H	5.10785600	10.83040700	0.00000000
H	14.94155800	-3.79667700	0.00000000
H	14.94165600	3.79611600	0.00000000

Table S2, Structure 2

C	2.60581400	-7.29426500	0.00000000
C	3.44011500	-8.46751100	0.00000000
C	4.82760600	-8.30778900	0.00000000
C	5.47598300	-7.02585700	0.00000000
C	4.63665400	-5.85120600	0.00000000
C	3.21558500	-6.03841500	0.00000000
C	5.24148800	-4.59136500	0.00000000
C	6.62985900	-4.42890400	0.00000000
C	7.47156600	-5.60012500	0.00000000
C	8.89434500	-5.39606800	0.00000000
C	9.49245100	-4.13322800	0.00000000
C	8.65014300	-2.96484300	0.00000000
C	7.26519400	-3.14538900	0.00000000
C	6.86582400	-6.86135800	0.00000000
C	9.02503900	-1.58777400	0.00000000
C	7.95332500	-0.72407400	0.00000000
C	10.92440500	-4.20223400	0.00000000
C	11.39083400	-5.48198700	0.00000000
C	1.18185900	-7.21346100	0.00000000
C	0.69865800	-5.92585900	0.00000000
C	3.04373400	-9.84533000	0.00000000
C	4.10523500	-10.69867000	0.00000000
S	5.63346200	-9.86340600	0.00000000
S	2.02003500	-4.75834800	0.00000000
S	6.43151500	-1.61185000	0.00000000
S	10.10795600	-6.65950700	0.00000000
H	4.60973000	-3.70670400	0.00000000
H	7.49761600	-7.74614500	0.00000000
H	10.05400000	-1.24619400	0.00000000
H	11.57264000	-3.33305900	0.00000000
H	0.53345100	-8.08289500	0.00000000
H	2.01224400	-10.17950100	0.00000000
C	-3.44888800	2.96467100	0.00000000
C	-2.59809400	4.12952900	0.00000000
C	-3.19396900	5.39354400	0.00000000
C	-4.61199800	5.60519200	0.00000000
C	-5.46407100	4.44107300	0.00000000
C	-4.83414200	3.15290900	0.00000000
C	-6.85135200	4.62123800	0.00000000
C	-7.44211200	5.88900500	0.00000000
C	-6.58940500	7.05366100	0.00000000
C	-7.21772200	8.34519500	0.00000000

C	-8.60213300	8.52466200	0.00000000
C	-9.45202300	7.36417000	0.00000000
C	-8.86313300	6.09833700	0.00000000
C	-5.20258800	6.87324000	0.00000000
C	-10.88486600	7.30512000	0.00000000
C	-11.35937500	6.02850100	0.00000000
C	-8.97825500	9.90857700	0.00000000
C	-7.90465000	10.74648500	0.00000000
C	-3.08048900	1.58582100	0.00000000
C	-4.15518800	0.72494600	0.00000000
C	-1.17261400	4.19569400	0.00000000
C	-0.67637600	5.47870800	0.00000000
S	-1.98564600	6.65901600	0.00000000
S	-5.67319200	1.62090900	0.00000000
S	-10.08448400	4.84192900	0.00000000
S	-6.38853900	9.88904300	0.00000000
H	-7.49426300	3.74454000	0.00000000
H	-4.56072300	7.75069300	0.00000000
H	-11.52718600	8.17863400	0.00000000
H	-10.00484800	10.25754400	0.00000000
H	-2.05273400	1.24060100	0.00000000
H	-0.53248300	3.32003900	0.00000000
C	-9.45215800	-7.36409500	0.00000000
C	-8.60229600	-8.52460000	0.00000000
C	-7.21787100	-8.34517200	0.00000000
C	-6.58951800	-7.05364400	0.00000000
C	-7.44221400	-5.88896700	0.00000000
C	-8.86325400	-6.09827900	0.00000000
C	-6.85148000	-4.62120000	0.00000000
C	-5.46419200	-4.44104500	0.00000000
C	-4.61214200	-5.60519200	0.00000000
C	-3.19409000	-5.39357400	0.00000000
C	-2.59822500	-4.12957500	0.00000000
C	-3.44896900	-2.96469200	0.00000000
C	-4.83424500	-3.15288300	0.00000000
C	-5.20271500	-6.87323800	0.00000000
C	-3.08053400	-1.58585400	0.00000000
C	-4.15519100	-0.72493700	0.00000000
C	-1.17270500	-4.19571600	0.00000000
C	-0.67637600	-5.47865700	0.00000000
C	-10.88499500	-7.30504500	0.00000000
C	-11.35951200	-6.02842000	0.00000000
C	-8.97844900	-9.90851200	0.00000000
C	-7.90487400	-10.74645600	0.00000000
S	-6.38873700	-9.88905800	0.00000000
S	-10.08459700	-4.84185900	0.00000000
S	-5.67323600	-1.62084700	0.00000000
S	-1.98574100	-6.65904300	0.00000000
H	-7.49440000	-3.74451300	0.00000000
H	-4.56083700	-7.75068300	0.00000000
H	-2.05276200	-1.24066700	0.00000000
H	-0.53264500	-3.32001000	0.00000000
H	-11.52729600	-8.17857200	0.00000000
H	-10.00505700	-10.25741200	0.00000000
C	8.65014400	2.96481300	0.00000000
C	9.49244700	4.13319900	0.00000000
C	8.89432200	5.39603300	0.00000000
C	7.47155400	5.60010300	0.00000000
C	6.62985000	4.42888000	0.00000000
C	7.26520300	3.14538200	0.00000000
C	5.24147600	4.59132400	0.00000000
C	4.63661700	5.85116800	0.00000000
C	5.47593700	7.02581200	0.00000000
C	4.82757600	8.30774400	0.00000000
C	3.44010100	8.46749900	0.00000000
C	2.60578700	7.29426900	0.00000000

C	3.21556600	6.03840100	0.00000000
C	6.86578400	6.86132300	0.00000000
C	1.18186000	7.21344000	0.00000000
C	0.69871900	5.92578800	0.00000000
C	3.04374800	9.84533300	0.00000000
C	4.10527100	10.69864300	0.00000000
C	9.02501300	1.58775100	0.00000000
C	7.95325200	0.72407900	0.00000000
C	10.92439700	4.20224100	0.00000000
C	11.39079700	5.48200400	0.00000000
S	10.10792200	6.65950200	0.00000000
S	6.43150200	1.61184000	0.00000000
S	2.02004700	4.75831500	0.00000000
S	5.63347800	9.86333700	0.00000000
H	4.60971000	3.70666500	0.00000000
H	7.49755400	7.74613000	0.00000000
H	0.53341600	8.08284900	0.00000000
H	2.01226600	10.17954200	0.00000000
H	10.05394900	1.24610500	0.00000000
H	11.57267100	3.33309500	0.00000000
H	-7.90464900	11.82832300	0.00000000
H	-12.39070900	5.70173900	0.00000000
H	-12.39083300	-5.70163200	0.00000000
H	-7.90487900	-11.82829600	0.00000000
H	4.08947800	-11.78037000	0.00000000
H	12.41999800	-5.81543400	0.00000000
H	12.41996100	5.81542900	0.00000000
H	4.08954800	11.78034300	0.00000000

Table S2, Structure 3

C	3.66674600	-7.88873300	0.00000000
C	3.47005100	-6.46498200	0.00000000
C	2.17182500	-5.94664800	0.00000000
C	0.99982900	-6.77874800	0.00000000
C	1.20178500	-8.21060400	0.00000000
C	2.54537500	-8.71408700	0.00000000
C	0.08669800	-9.05005100	0.00000000
C	-1.22060100	-8.56196900	0.00000000
C	-1.43257500	-7.13222000	0.00000000
C	-2.79187900	-6.66699200	0.00000000
C	-3.89317500	-7.52893300	0.00000000
C	-3.67736400	-8.95057200	0.00000000
C	-2.36783000	-9.42445500	0.00000000
C	-0.31332400	-6.28791000	0.00000000
C	-4.64833700	-10.00573100	0.00000000
C	-4.07870600	-11.24277900	0.00000000
C	-5.13612300	-6.84093100	0.00000000
C	-5.01684100	-5.47085200	0.00000000
C	4.89740900	-8.62490500	0.00000000
C	4.70131700	-9.97253700	0.00000000
C	4.46941100	-5.45549100	0.00000000
C	3.97397700	-4.17367900	0.00000000
S	2.20893200	-4.18874200	0.00000000
S	3.01316800	-10.40273500	0.00000000
S	-2.33813900	-11.17667200	0.00000000
S	-3.31994100	-4.99358500	0.00000000
H	0.24281200	-10.12587600	0.00000000
H	-0.46946100	-5.21171500	0.00000000
H	-5.72054600	-9.84506500	0.00000000
H	-6.09386600	-7.34735000	0.00000000
H	5.88014900	-8.16694600	0.00000000
H	5.53125300	-5.67395700	0.00000000
C	12.93564900	-0.71920600	0.00000000

C	12.93565100	0.71936000	0.00000000
C	11.71288200	1.39269800	0.00000000
C	10.44261600	0.72198700	0.00000000
C	10.44261500	-0.72183900	0.00000000
C	11.71288200	-1.39254800	0.00000000
C	9.21737400	-1.39547700	0.00000000
C	7.99209800	-0.71961400	0.00000000
C	7.99209800	0.71977100	0.00000000
C	6.72204600	1.38247100	0.00000000
C	5.48873500	0.72234200	0.00000000
C	5.48873200	-0.72219400	0.00000000
C	6.72204700	-1.38231500	0.00000000
C	9.21737400	1.39562900	0.00000000
C	4.38323900	-1.63198600	0.00000000
C	4.75691500	-2.95633000	0.00000000
C	4.38323800	1.63212800	0.00000000
C	4.75689900	2.95647400	0.00000000
C	14.05703400	-1.61317700	0.00000000
C	13.68608900	-2.92360100	0.00000000
C	14.05703500	1.61333600	0.00000000
C	13.68608200	2.92375700	0.00000000
S	11.95639100	3.12800100	0.00000000
S	11.95640100	-3.12785200	0.00000000
S	6.51419000	-3.11318800	0.00000000
S	6.51418000	3.11334500	0.00000000
H	9.21821500	-2.48257700	0.00000000
H	9.21822100	2.48272900	0.00000000
H	3.34553900	-1.31539900	0.00000000
H	3.34554200	1.31553000	0.00000000
H	15.09126600	-1.28754700	0.00000000
H	15.09126800	1.28771100	0.00000000
C	3.46997200	6.46509900	0.00000000
C	3.66662000	7.88885700	0.00000000
C	2.54522700	8.71418400	0.00000000
C	1.20165000	8.21066500	0.00000000
C	0.99974200	6.77879900	0.00000000
C	2.17176200	5.94673300	0.00000000
C	-0.31339600	6.28791600	0.00000000
C	-1.43267300	7.13218900	0.00000000
C	-1.22074600	8.56194700	0.00000000
C	-2.36800300	9.42440100	0.00000000
C	-3.67752200	8.95047500	0.00000000
C	-3.89328400	7.52883200	0.00000000
C	-2.79196200	6.66691900	0.00000000
C	0.08653900	9.05007400	0.00000000
C	-5.13621500	6.84080500	0.00000000
C	-5.01690900	5.47072600	0.00000000
C	-4.64853200	10.00560100	0.00000000
C	-4.07894000	11.24266700	0.00000000
C	4.46936400	5.45563600	0.00000000
C	3.97395200	4.17381400	0.00000000
C	4.89726000	8.62505500	0.00000000
C	4.70114000	9.97268600	0.00000000
S	3.01298400	10.40284400	0.00000000
S	2.20890700	4.18883100	0.00000000
S	-3.31999400	4.99350100	0.00000000
S	-2.33837000	11.17661900	0.00000000
H	-0.46950600	5.21171900	0.00000000
H	0.24261600	10.12590500	0.00000000
H	-6.09395800	7.34722300	0.00000000
H	-5.72073500	9.84489400	0.00000000
H	5.53120300	5.67412700	0.00000000
H	5.88001000	8.16711700	0.00000000
C	-8.31761200	3.71928800	0.00000000
C	-9.75588800	3.71232100	0.00000000
C	-10.41634700	2.48556700	0.00000000

C	-9.73135200	1.22411700	0.00000000
C	-8.28626800	1.22778100	0.00000000
C	-7.62716700	2.50357900	0.00000000
C	-7.61163800	-0.00008400	0.00000000
C	-8.28626500	-1.22795700	0.00000000
C	-9.73134700	-1.22430100	0.00000000
C	-10.41633300	-2.48575300	0.00000000
C	-9.75586100	-3.71250400	0.00000000
C	-8.31758500	-3.71946100	0.00000000
C	-7.62715100	-2.50374600	0.00000000
C	-10.40277400	-0.00009400	0.00000000
C	-7.45296800	-4.84710400	0.00000000
C	-6.11533000	-4.52595000	0.00000000
C	-10.65831900	-4.82684900	0.00000000
C	-11.96531100	-4.44390300	0.00000000
C	-7.45301300	4.84693400	0.00000000
C	-6.11536600	4.52578900	0.00000000
C	-10.65835700	4.82666000	0.00000000
C	-11.96534400	4.44370000	0.00000000
S	-12.15392300	2.71211900	0.00000000
S	-5.89433400	2.77749400	0.00000000
S	-5.89431900	-2.77764100	0.00000000
S	-12.15390800	-2.71232500	0.00000000
H	-6.52425000	-0.00008500	0.00000000
H	-11.48988500	-0.00009500	0.00000000
H	-7.81212600	-5.86923300	0.00000000
H	-10.34291000	-5.86419800	0.00000000
H	-7.81217700	5.86906100	0.00000000
H	-10.34296200	5.86401300	0.00000000
H	5.44956000	-10.75392600	0.00000000
H	-4.57488100	-12.20416100	0.00000000
H	-12.84387200	-5.07521800	0.00000000
H	-12.84390400	5.07501000	0.00000000
H	-4.57514500	12.20403300	0.00000000
H	5.44937200	10.75408500	0.00000000
H	14.32543000	3.79649200	0.00000000
H	14.32543900	-3.79633500	0.00000000

Table S2, Structure 4

C	-4.73872200	-6.44528000	0.00000000
C	-6.02580000	-7.09642300	0.00000000
C	-7.18863500	-6.31352600	0.00000000
C	-7.18309200	-4.87456400	0.00000000
C	-5.89292300	-4.23448600	0.00000000
C	-4.72113500	-5.05182700	0.00000000
C	-5.82315800	-2.84275800	0.00000000
C	-6.96333800	-2.04169200	0.00000000
C	-8.26155700	-2.66532600	0.00000000
C	-9.39952600	-1.78457800	0.00000000
C	-9.30150000	-0.38619500	0.00000000
C	-7.99648800	0.22815300	0.00000000
C	-6.88697800	-0.61502900	0.00000000
C	-8.33098700	-4.06708400	0.00000000
C	-7.62710000	1.61377100	0.00000000
C	-6.26614300	1.81980200	0.00000000
C	-10.58461000	0.25276500	0.00000000
C	-11.61826800	-0.63439800	0.00000000
C	-3.41898100	-7.00629200	0.00000000
C	-2.41951000	-6.05988900	0.00000000
C	-6.31140700	-8.50108800	0.00000000
C	-7.64673300	-8.77023800	0.00000000
S	-8.61806100	-7.32553600	0.00000000
S	-3.09474000	-4.43053200	0.00000000

S	-5.39670400	0.28526800	0.00000000
S	-11.07677400	-2.28892400	0.00000000
H	-4.84664700	-2.36623400	0.00000000
H	-9.30820400	-4.54395200	0.00000000
H	-8.34368100	2.42833700	0.00000000
H	-10.72351500	1.32818700	0.00000000
H	-3.21742300	-8.07228800	0.00000000
H	-5.54909000	-9.27227500	0.00000000
C	-2.17045500	4.76894300	0.00000000
C	-3.55581800	4.38714500	0.00000000
C	-4.53925100	5.37560400	0.00000000
C	-4.22930300	6.77727700	0.00000000
C	-2.83348800	7.16452000	0.00000000
C	-1.84328200	6.12464200	0.00000000
C	-2.51503800	8.52626400	0.00000000
C	-3.49262900	9.52715100	0.00000000
C	-4.88303100	9.14116000	0.00000000
C	-5.86926100	10.18500300	0.00000000
C	-5.54770900	11.54361800	0.00000000
C	-4.16193600	11.92841200	0.00000000
C	-3.18578100	10.93009100	0.00000000
C	-5.20445400	7.77956600	0.00000000
C	-3.60026800	13.24794500	0.00000000
C	-2.23838700	13.24067600	0.00000000
C	-6.70942400	12.38462900	0.00000000
C	-7.87264200	11.67643900	0.00000000
C	-1.03174000	3.91806700	0.00000000
C	0.16676400	4.59256600	0.00000000
C	-4.09046400	3.07256600	0.00000000
C	-5.46418400	3.02456500	0.00000000
S	-6.14303000	4.65328000	0.00000000
S	-0.10129100	6.33669800	0.00000000
S	-1.57881600	11.62876200	0.00000000
S	-7.60655800	9.95503200	0.00000000
H	-1.46754700	8.81770500	0.00000000
H	-6.25212200	7.48876600	0.00000000
H	-4.19043900	14.15752900	0.00000000
H	-6.67265900	13.46828700	0.00000000
H	-1.09643100	2.83657700	0.00000000
H	-3.47243100	2.18223200	0.00000000
C	3.78816800	1.04775600	0.00000000
C	3.15615500	2.34206200	0.00000000
C	3.95843100	3.48468900	0.00000000
C	5.39283000	3.43730500	0.00000000
C	6.02738600	2.13776400	0.00000000
C	5.18256400	0.97758100	0.00000000
C	7.42431000	2.07149100	0.00000000
C	8.23019600	3.21504100	0.00000000
C	7.59702700	4.51179400	0.00000000
C	8.44368900	5.67178500	0.00000000
C	9.83821400	5.60317300	0.00000000
C	10.46922300	4.31078100	0.00000000
C	9.66554900	3.16909500	0.00000000
C	6.19965000	4.57959300	0.00000000
C	11.86901300	3.99889600	0.00000000
C	12.11008500	2.65850100	0.00000000
C	10.45342800	6.89862000	0.00000000
C	9.54496000	7.91322800	0.00000000
C	3.16949200	-0.23316000	0.00000000
C	4.05987100	-1.28302200	0.00000000
C	1.76565700	2.64216700	0.00000000
C	1.48550300	3.98992400	0.00000000
S	2.97288700	4.93470700	0.00000000
S	5.71959600	-0.69141200	0.00000000
S	10.64529100	1.71621500	0.00000000
S	7.90100300	7.33801200	0.00000000

H	7.90169400	1.09465300	0.00000000
H	5.72315900	5.55687500	0.00000000
H	12.65591000	4.74487800	0.00000000
H	11.52563400	7.05994900	0.00000000
H	2.09529600	-0.37517000	0.00000000
H	0.99288000	1.88263100	0.00000000
C	6.84434600	-10.61923400	0.00000000
C	5.68843300	-11.47496300	0.00000000
C	4.41953400	-10.89262700	0.00000000
C	4.20326100	-9.47294500	0.00000000
C	5.36297800	-8.61429000	0.00000000
C	6.65775200	-9.23553800	0.00000000
C	5.17539900	-7.22785500	0.00000000
C	3.90601300	-6.64102400	0.00000000
C	2.74198500	-7.50317600	0.00000000
C	1.44629900	-6.88517400	0.00000000
C	1.27183700	-5.50182200	0.00000000
C	2.42512500	-4.64458100	0.00000000
C	3.69521900	-5.22066400	0.00000000
C	2.93216100	-8.88856400	0.00000000
C	2.45480100	-3.22342800	0.00000000
C	3.72383700	-2.69343000	0.00000000
C	-0.09355200	-5.11483500	0.00000000
C	-0.97628400	-6.16846000	0.00000000
C	8.23019600	-10.98810000	0.00000000
C	9.06224800	-9.90991300	0.00000000
C	5.63678200	-12.90821400	0.00000000
C	4.36286100	-13.38961600	0.00000000
S	3.16949200	-12.12080500	0.00000000
S	8.19707100	-8.39830400	0.00000000
S	4.93397300	-3.97768400	0.00000000
S	-0.10957400	-7.70549000	0.00000000
H	6.04965200	-6.58147000	0.00000000
H	2.05833000	-9.53553300	0.00000000
H	1.56242400	-2.60905200	0.00000000
H	-0.41561400	-4.07997700	0.00000000
H	8.58431300	-12.01292800	0.00000000
H	6.51369000	-13.54595300	0.00000000
H	-1.56823200	14.09000600	0.00000000
H	-8.88472000	12.05873800	0.00000000
H	-12.67878400	-0.42064800	0.00000000
H	-8.13057600	-9.73785200	0.00000000
H	13.06733800	2.15439800	0.00000000
H	4.04160900	-14.42269300	0.00000000
H	10.14410500	-9.90401800	0.00000000
H	9.73633100	8.97804900	0.00000000

Table S2, Structure 5

C	-3.91216100	-9.14692800	0.00000000
C	-2.88332200	-8.14462700	0.00000000
C	-3.22297000	-6.78715700	0.00000000
C	-4.58851600	-6.33049600	0.00000000
C	-5.61870600	-7.34698900	0.00000000
C	-5.23734000	-8.72914400	0.00000000
C	-6.95561100	-6.95552800	0.00000000
C	-7.34726900	-5.61871800	0.00000000
C	-6.33091900	-4.58833800	0.00000000
C	-6.78775000	-3.22286700	0.00000000
C	-8.14527700	-2.88336600	0.00000000
C	-9.14742700	-3.91239900	0.00000000
C	-8.72948200	-5.23751500	0.00000000
C	-4.98256300	-4.98218000	0.00000000
C	-10.57545100	-3.77982900	0.00000000

C	-11.21213800	-4.98358900	0.00000000
C	-8.37099500	-1.48573500	0.00000000
C	-7.22506200	-0.72586700	0.00000000
C	-3.77943600	-10.57493800	0.00000000
C	-4.98311200	-11.21178100	0.00000000
C	-1.48562800	-8.37003500	0.00000000
C	-0.72596400	-7.22406600	0.00000000
S	-1.76527200	-5.79823600	0.00000000
S	-6.32655700	-10.10236500	0.00000000
S	-10.10257100	-6.32690600	0.00000000
S	-5.79922400	-1.76490000	0.00000000
H	-7.72413400	-7.72417900	0.00000000
H	-4.21354200	-4.21308500	0.00000000
H	-11.09963600	-2.83082700	0.00000000
H	-9.36391000	-1.05505400	0.00000000
H	-2.83039200	-11.09904600	0.00000000
H	-1.05469000	-9.36285200	0.00000000
C	9.14750900	-3.91257500	0.00000000
C	8.14541700	-2.88355600	0.00000000
C	6.78790800	-3.22300500	0.00000000
C	6.33092300	-4.58846800	0.00000000
C	7.34724800	-5.61882200	0.00000000
C	8.72946600	-5.23769000	0.00000000
C	6.95560600	-6.95567200	0.00000000
C	5.61873700	-7.34710400	0.00000000
C	4.58851100	-6.33058400	0.00000000
C	3.22296200	-6.78725900	0.00000000
C	2.88328000	-8.14472000	0.00000000
C	3.91213300	-9.14701500	0.00000000
C	5.23731000	-8.72925400	0.00000000
C	4.98254100	-4.98228600	0.00000000
C	3.77936900	-10.57501800	0.00000000
C	4.98302800	-11.21190200	0.00000000
C	1.48558300	-8.37011200	0.00000000
C	0.72597000	-7.22409600	0.00000000
C	10.57552700	-3.78015300	0.00000000
C	11.21213700	-4.98396200	0.00000000
C	8.37099400	-1.48587300	0.00000000
C	7.22513600	-0.72602300	0.00000000
S	5.79921400	-1.76521600	0.00000000
S	10.10245700	-6.32717300	0.00000000
S	6.32647500	-10.10250800	0.00000000
S	1.76529100	-5.79833000	0.00000000
H	7.72414900	-7.72430600	0.00000000
H	4.21356700	-4.21314500	0.00000000
H	2.83030100	-11.09908700	0.00000000
H	1.05458900	-9.36290200	0.00000000
H	11.09985500	-2.83122700	0.00000000
H	9.36390800	-1.05518200	0.00000000
C	3.91212700	9.14697000	0.00000000
C	2.88329000	8.14467500	0.00000000
C	3.22295500	6.78721000	0.00000000
C	4.58851100	6.33055500	0.00000000
C	5.61869900	7.34705500	0.00000000
C	5.23731100	8.72919700	0.00000000
C	6.95560500	6.95561300	0.00000000
C	7.34726600	5.61881000	0.00000000
C	6.33093600	4.58841000	0.00000000
C	6.78781300	3.22294000	0.00000000
C	8.14533800	2.88344000	0.00000000
C	9.14743900	3.91249100	0.00000000
C	8.72947100	5.23759500	0.00000000
C	4.98256600	4.98223500	0.00000000
C	10.57546100	3.77993400	0.00000000
C	11.21215100	4.98369400	0.00000000
C	8.37094700	1.48578900	0.00000000

C	7.22499600	0.72598800	0.00000000
C	3.77939500	10.57497600	0.00000000
C	4.98306300	11.21183600	0.00000000
C	1.48559100	8.37006700	0.00000000
C	0.72594800	7.22408600	0.00000000
S	1.76527600	5.79826900	0.00000000
S	6.32651000	10.10242900	0.00000000
S	10.10255700	6.32698300	0.00000000
S	5.79922600	1.76504100	0.00000000
H	7.72411400	7.72427800	0.00000000
H	4.21355100	4.21313400	0.00000000
H	11.09964800	2.83093100	0.00000000
H	9.36381300	1.05505000	0.00000000
H	2.83034300	11.09907300	0.00000000
H	1.05463000	9.36287300	0.00000000
C	-9.14747700	3.91244500	0.00000000
C	-8.14529300	2.88345300	0.00000000
C	-6.78784300	3.22295400	0.00000000
C	-6.33089900	4.58839000	0.00000000
C	-7.34726500	5.61872400	0.00000000
C	-8.72947600	5.23756500	0.00000000
C	-6.95563600	6.95558400	0.00000000
C	-5.61877500	7.34703900	0.00000000
C	-4.58853200	6.33052500	0.00000000
C	-3.22298500	6.78721900	0.00000000
C	-2.88332200	8.14468200	0.00000000
C	-3.91218800	9.14697100	0.00000000
C	-5.23735600	8.72919800	0.00000000
C	-4.98253300	4.98224100	0.00000000
C	-3.77943300	10.57497500	0.00000000
C	-4.98310200	11.21184500	0.00000000
C	-1.48562900	8.37008400	0.00000000
C	-0.72599000	7.22408200	0.00000000
C	-10.57547400	3.77996600	0.00000000
C	-11.21213200	4.98375400	0.00000000
C	-8.37081300	1.48584800	0.00000000
C	-7.22515700	0.72592100	0.00000000
S	-5.79894400	1.76527300	0.00000000
S	-10.10250400	6.32700400	0.00000000
S	-6.32654000	10.10243900	0.00000000
S	-1.76529600	5.79831100	0.00000000
H	-7.72419500	7.72420000	0.00000000
H	-4.21354700	4.21310600	0.00000000
H	-2.83036900	11.09904900	0.00000000
H	-1.05464000	9.36287600	0.00000000
H	-11.09980100	2.83103400	0.00000000
H	-9.36363100	1.05491300	0.00000000
H	12.27722900	-5.17375700	0.00000000
H	12.27725500	5.17341900	0.00000000
H	5.17264000	12.27696800	0.00000000
H	-5.17266100	12.27698000	0.00000000
H	-12.27723600	5.17347600	0.00000000
H	-12.27724300	-5.17330500	0.00000000
H	5.17257700	-12.27703900	0.00000000
H	-5.17270000	-12.27691100	0.00000000

Table S2, Structure 6

C	2.86898500	3.88256100	0.00000000
C	3.88256100	2.86898500	0.00000000
C	5.22549800	3.23273200	0.00000000
C	5.63855900	4.61021700	0.00000000
C	4.61021700	5.63855900	0.00000000
C	3.23273200	5.22549800	0.00000000

C	5.00559300	6.97929300	0.00000000
C	6.34961300	7.36960100	0.00000000
C	7.36960100	6.34961300	0.00000000
C	8.74186200	6.77260300	0.00000000
C	9.13071800	8.11386400	0.00000000
C	8.11386400	9.13071800	0.00000000
C	6.77260300	8.74186200	0.00000000
C	6.97929300	5.00559300	0.00000000
C	8.27372600	10.55599200	0.00000000
C	7.08423900	11.21942400	0.00000000
C	10.55599200	8.27372600	0.00000000
C	11.21942400	7.08423900	0.00000000
C	1.47028700	3.67601300	0.00000000
C	0.72696800	4.83214700	0.00000000
C	3.67601300	1.47028700	0.00000000
C	4.83214700	0.72696800	0.00000000
S	6.24235400	1.79084200	0.00000000
S	1.79084200	6.24235400	0.00000000
S	5.71727100	10.14056300	0.00000000
S	10.14056300	5.71727100	0.00000000
H	4.23679400	7.74831700	0.00000000
H	7.74831700	4.23679400	0.00000000
H	9.23472200	11.05808700	0.00000000
H	11.05808700	9.23472200	0.00000000
H	1.02614200	2.68986200	0.00000000
H	2.68986200	1.02614200	0.00000000
C	-9.13071800	-8.11386400	0.00000000
C	-8.11386400	-9.13071800	0.00000000
C	-6.77260300	-8.74186200	0.00000000
C	-6.34961300	-7.36960100	0.00000000
C	-7.36960100	-6.34961300	0.00000000
C	-8.74186200	-6.77260300	0.00000000
C	-6.97929300	-5.00559300	0.00000000
C	-5.63855900	-4.61021700	0.00000000
C	-4.61021700	-5.63855900	0.00000000
C	-3.23273200	-5.22549800	0.00000000
C	-2.86898500	-3.88256100	0.00000000
C	-3.88256100	-2.86898500	0.00000000
C	-5.22549800	-3.23273200	0.00000000
C	-5.00559300	-6.97929300	0.00000000
C	-3.67601300	-1.47028700	0.00000000
C	-4.83214700	-0.72696800	0.00000000
C	-1.47028700	-3.67601300	0.00000000
C	-0.72696800	-4.83214700	0.00000000
C	-10.55599200	-8.27372600	0.00000000
C	-11.21942400	-7.08423900	0.00000000
C	-8.27372600	-10.55599200	0.00000000
C	-7.08423900	-11.21942400	0.00000000
S	-5.71727100	-10.14056300	0.00000000
S	-10.14056300	-5.71727100	0.00000000
S	-6.24235400	-1.79084200	0.00000000
S	-1.79084200	-6.24235400	0.00000000
H	-7.74831700	-4.23679400	0.00000000
H	-4.23679400	-7.74831700	0.00000000
H	-2.68986200	-1.02614200	0.00000000
H	-1.02614200	-2.68986200	0.00000000
H	-11.05808700	-9.23472200	0.00000000
H	-9.23472200	-11.05808700	0.00000000
C	-3.88256100	2.86898500	0.00000000
C	-2.86898500	3.88256100	0.00000000
C	-3.23273200	5.22549800	0.00000000
C	-4.61021700	5.63855900	0.00000000
C	-5.63855900	4.61021700	0.00000000
C	-5.22549800	3.23273200	0.00000000
C	-6.97929300	5.00559300	0.00000000
C	-7.36960100	6.34961300	0.00000000

C	-6.34961300	7.36960100	0.00000000
C	-6.77260300	8.74186200	0.00000000
C	-8.11386400	9.13071800	0.00000000
C	-9.13071800	8.11386400	0.00000000
C	-8.74186200	6.77260300	0.00000000
C	-5.00559300	6.97929300	0.00000000
C	-10.55599200	8.27372600	0.00000000
C	-11.21942400	7.08423900	0.00000000
C	-8.27372600	10.55599200	0.00000000
C	-7.08423900	11.21942400	0.00000000
C	-3.67601300	1.47028700	0.00000000
C	-4.83214700	0.72696800	0.00000000
C	-1.47028700	3.67601300	0.00000000
C	-0.72696800	4.83214700	0.00000000
S	-1.79084200	6.24235400	0.00000000
S	-6.24235400	1.79084200	0.00000000
S	-10.14056300	5.71727100	0.00000000
S	-5.71727100	10.14056300	0.00000000
H	-7.74831700	4.23679400	0.00000000
H	-4.23679400	7.74831700	0.00000000
H	-11.05808700	9.23472200	0.00000000
H	-9.23472200	11.05808700	0.00000000
H	-2.68986200	1.02614200	0.00000000
H	-1.02614200	2.68986200	0.00000000
C	8.11386400	-9.13071800	0.00000000
C	9.13071800	-8.11386400	0.00000000
C	8.74186200	-6.77260300	0.00000000
C	7.36960100	-6.34961300	0.00000000
C	6.34961300	-7.36960100	0.00000000
C	6.77260300	-8.74186200	0.00000000
C	5.00559300	-6.97929300	0.00000000
C	4.61021700	-5.63855900	0.00000000
C	5.63855900	-4.61021700	0.00000000
C	5.22549800	-3.23273200	0.00000000
C	3.88256100	-2.86898500	0.00000000
C	2.86898500	-3.88256100	0.00000000
C	3.23273200	-5.22549800	0.00000000
C	6.97929300	-5.00559300	0.00000000
C	1.47028700	-3.67601300	0.00000000
C	0.72696800	-4.83214700	0.00000000
C	3.67601300	-1.47028700	0.00000000
C	4.83214700	-0.72696800	0.00000000
C	8.27372600	-10.55599200	0.00000000
C	7.08423900	-11.21942400	0.00000000
C	10.55599200	-8.27372600	0.00000000
C	11.21942400	-7.08423900	0.00000000
S	10.14056300	-5.71727100	0.00000000
S	5.71727100	-10.14056300	0.00000000
S	1.79084200	-6.24235400	0.00000000
S	6.24235400	-1.79084200	0.00000000
H	4.23679400	-7.74831700	0.00000000
H	7.74831700	-4.23679400	0.00000000
H	1.02614200	-2.68986200	0.00000000
H	2.68986200	-1.02614200	0.00000000
H	9.23472200	-11.05808700	0.00000000
H	11.05808700	-9.23472200	0.00000000
H	-12.28868100	6.91927600	0.00000000
H	-6.91927600	12.28868100	0.00000000
H	6.91927600	12.28868100	0.00000000
H	12.28868100	6.91927600	0.00000000
H	12.28868100	-6.91927600	0.00000000
H	6.91927600	-12.28868100	0.00000000
H	-6.91927600	-12.28868100	0.00000000
H	-12.28868100	-6.91927600	0.00000000

Table S2, Structure 7

C	0.29709500	7.99015200	0.00000000
C	-0.40671300	6.72973300	0.00000000
C	0.36496100	5.56854100	0.00000000
C	1.79409500	5.54758900	0.00000000
C	2.50506900	6.79908100	0.00000000
C	1.70007800	7.99315500	0.00000000
C	3.90919200	6.77094500	0.00000000
C	4.63560400	5.56900800	0.00000000
C	3.90726000	4.32750800	0.00000000
C	4.63984200	3.10029700	0.00000000
C	6.03128400	3.01259200	0.00000000
C	6.77099500	4.25229200	0.00000000
C	6.07221100	5.46877400	0.00000000
C	2.51400500	4.35449100	0.00000000
C	8.19226200	4.43873600	0.00000000
C	8.55563900	5.75180200	0.00000000
C	6.49215000	1.65371900	0.00000000
C	5.47131400	0.72690400	0.00000000
C	-0.25191700	9.31420800	0.00000000
C	0.70358500	10.28536100	0.00000000
C	-1.81391300	6.44934300	0.00000000
C	-2.10614200	5.10182800	0.00000000
S	-0.62601200	4.14309400	0.00000000
S	2.31669300	9.63219700	0.00000000
S	7.18337000	6.82224500	0.00000000
S	3.90096600	1.52945400	0.00000000
H	4.45277200	7.71286000	0.00000000
H	1.97064300	3.41349900	0.00000000
H	8.90773900	3.62387000	0.00000000
H	7.54022900	1.37474000	0.00000000
H	-1.31530400	9.52667700	0.00000000
H	-2.57965900	7.21746800	0.00000000
C	-7.06822200	-3.73778400	0.00000000
C	-5.62476300	-3.71709000	0.00000000
C	-5.00497800	-2.46820400	0.00000000
C	-5.70140100	-1.22006300	0.00000000
C	-7.14071100	-1.23008700	0.00000000
C	-7.77231400	-2.52426700	0.00000000
C	-7.81840600	-0.00001300	0.00000000
C	-7.14070400	1.23004700	0.00000000
C	-5.70136200	1.22003300	0.00000000
C	-5.00485800	2.46807300	0.00000000
C	-5.62462300	3.71694900	0.00000000
C	-7.06809000	3.73770800	0.00000000
C	-7.77220200	2.52430200	0.00000000
C	-5.02810200	-0.00005400	0.00000000
C	-7.94019000	4.87533900	0.00000000
C	-9.25902600	4.53350000	0.00000000
C	-4.67823800	4.79550700	0.00000000
C	-3.36517400	4.37484500	0.00000000
C	-7.94038300	-4.87527000	0.00000000
C	-9.25917700	-4.53335800	0.00000000
C	-4.67833800	-4.79556600	0.00000000
C	-3.36524100	-4.37488600	0.00000000
S	-3.27501800	-2.61368900	0.00000000
S	-9.50007400	-2.80978300	0.00000000
S	-9.49992200	2.80985900	0.00000000
S	-3.27502900	2.61360800	0.00000000
H	-8.90591900	-0.00021700	0.00000000
H	-3.94149800	-0.00012300	0.00000000
H	-7.59223300	5.90239400	0.00000000
H	-4.96067400	5.84266000	0.00000000
H	-7.59269300	-5.90242500	0.00000000

H	-4.96068100	-5.84278400	0.00000000
C	-0.40666100	-6.72954100	0.00000000
C	0.29709500	-7.99000000	0.00000000
C	1.69999100	-7.99307600	0.00000000
C	2.50510000	-6.79905500	0.00000000
C	1.79410200	-5.54754000	0.00000000
C	0.36501500	-5.56837000	0.00000000
C	2.51409800	-4.35443800	0.00000000
C	3.90730600	-4.32752700	0.00000000
C	4.63564200	-5.56899400	0.00000000
C	6.07223700	-5.46888800	0.00000000
C	6.77112700	-4.25236800	0.00000000
C	6.03147600	-3.01264300	0.00000000
C	4.64001700	-3.10033600	0.00000000
C	3.90921500	-6.77093200	0.00000000
C	6.49225100	-1.65377600	0.00000000
C	5.47138300	-0.72694100	0.00000000
C	8.19229900	-4.43893800	0.00000000
C	8.55559200	-5.75200300	0.00000000
C	-1.81391200	-6.44922600	0.00000000
C	-2.10614000	-5.10174900	0.00000000
C	-0.25207300	-9.31407600	0.00000000
C	0.70338700	-10.28530200	0.00000000
S	2.31655200	-9.63210300	0.00000000
S	-0.62593700	-4.14306300	0.00000000
S	3.90103000	-1.52940400	0.00000000
S	7.18338100	-6.82241400	0.00000000
H	1.97085500	-3.41337600	0.00000000
H	4.45314700	-7.71264300	0.00000000
H	7.54034000	-1.37468400	0.00000000
H	8.90799700	-3.62425200	0.00000000
H	-2.57955500	-7.21740000	0.00000000
H	-1.31550700	-9.52626300	0.00000000
H	-10.11689500	5.19264400	0.00000000
H	0.56157500	11.35783800	0.00000000
H	9.55540900	6.16516700	0.00000000
H	9.55538900	-6.16525700	0.00000000
H	0.56148600	-11.35781000	0.00000000
H	-10.11696400	-5.19258100	0.00000000

Table S2, Structure 8

C	-3.44020900	0.71656000	0.00000000
C	-3.44021300	-0.71651900	0.00000000
C	-4.64224000	-1.41390700	0.00000000
C	-5.90740600	-0.72841200	0.00000000
C	-5.90743900	0.72846900	0.00000000
C	-4.64223100	1.41394900	0.00000000
C	-7.13581900	1.39536800	0.00000000
C	-8.36226100	0.72110700	0.00000000
C	-8.36223500	-0.72114200	0.00000000
C	-9.63149700	-1.39238300	0.00000000
C	-10.85476900	-0.71913100	0.00000000
C	-10.85483100	0.71887800	0.00000000
C	-9.63161600	1.39222500	0.00000000
C	-7.13575400	-1.39535800	0.00000000
C	-11.97596600	1.61325200	0.00000000
C	-11.60457400	2.92352600	0.00000000
C	-11.97583400	-1.61359800	0.00000000
C	-11.60432900	-2.92383500	0.00000000
C	-2.30226100	1.55407200	0.00000000
C	-2.57753200	2.90078400	0.00000000
C	-2.30226100	-1.55403400	0.00000000
C	-2.57753200	-2.90074100	0.00000000
S	-4.33050000	-3.15574600	0.00000000

S	-4.33048900	3.15578100	0.00000000
S	-9.87480000	3.12771500	0.00000000
S	-9.87453100	-3.12790300	0.00000000
H	-7.13606600	2.48269600	0.00000000
H	-7.13596000	-2.48266300	0.00000000
H	-13.01026800	1.28792700	0.00000000
H	-13.01016000	-1.28835000	0.00000000
H	-1.29447700	1.15957400	0.00000000
H	-1.29448100	-1.15952600	0.00000000
C	7.31414700	4.40133900	0.00000000
C	6.73462400	3.07329700	0.00000000
C	5.34593600	3.02784400	0.00000000
C	4.47554400	4.15456100	0.00000000
C	5.02845600	5.47738500	0.00000000
C	6.47192500	5.53344700	0.00000000
C	4.13295200	6.56691800	0.00000000
C	2.73318600	6.38937200	0.00000000
C	2.21669800	5.04885900	0.00000000
C	0.80778100	4.83028600	0.00000000
C	-0.15347500	5.83399200	0.00000000
C	0.34428800	7.19304700	0.00000000
C	1.73340900	7.42968900	0.00000000
C	3.09861300	3.97814500	0.00000000
C	-0.41257000	8.40983600	0.00000000
C	0.36908700	9.52592600	0.00000000
C	-1.49298300	5.29569900	0.00000000
C	-1.53338200	3.91621500	0.00000000
C	8.70128700	4.75950500	0.00000000
C	8.90727300	6.10661000	0.00000000
C	7.31499800	1.74836200	0.00000000
C	6.37533500	0.73291000	0.00000000
S	4.74697500	1.41680600	0.00000000
S	7.41864700	7.00591200	0.00000000
S	2.06727700	9.14820200	0.00000000
S	0.10165300	3.25001000	0.00000000
H	4.53332300	7.57807300	0.00000000
H	2.69784000	2.96944800	0.00000000
H	-1.49648700	8.44322500	0.00000000
H	-2.38784600	5.90920200	0.00000000
H	9.50801700	4.03473400	0.00000000
H	8.38377400	1.56239500	0.00000000
C	6.73462500	-3.07325900	0.00000000
C	7.31414700	-4.40130000	0.00000000
C	6.47192500	-5.53340800	0.00000000
C	5.02845500	-5.47734700	0.00000000
C	4.47554400	-4.15452200	0.00000000
C	5.34593700	-3.02780500	0.00000000
C	3.09861400	-3.97810500	0.00000000
C	2.21669900	-5.04881800	0.00000000
C	2.73318500	-6.38933200	0.00000000
C	1.73340700	-7.42964800	0.00000000
C	0.34428500	-7.19300400	0.00000000
C	-0.15347500	-5.83394900	0.00000000
C	0.80778200	-4.83024300	0.00000000
C	4.13295100	-6.56687900	0.00000000
C	-1.49298200	-5.29565200	0.00000000
C	-1.53337800	-3.91616700	0.00000000
C	-0.41257400	-8.40979100	0.00000000
C	0.36908100	-9.52588300	0.00000000
C	7.31499900	-1.74832300	0.00000000
C	6.37533500	-0.73287100	0.00000000
C	8.70128700	-4.75946700	0.00000000
C	8.90727200	-6.10657300	0.00000000
S	7.41864600	-7.00587400	0.00000000
S	4.74697600	-1.41676700	0.00000000
S	0.10165900	-3.24996500	0.00000000

S	2.06727200	-9.14816100	0.00000000
H	2.69784200	-2.96940800	0.00000000
H	4.53332100	-7.57803400	0.00000000
H	-2.38784600	-5.90915300	0.00000000
H	-1.49649100	-8.44318000	0.00000000
H	8.38377400	-1.56235500	0.00000000
H	9.50801700	-4.03469700	0.00000000
H	0.05212400	10.56026400	0.00000000
H	-12.24373500	3.79639400	0.00000000
H	0.05211800	-10.56022000	0.00000000
H	9.85094200	-6.63555100	0.00000000
H	9.85094200	6.63558800	0.00000000
H	-12.24342800	-3.79674800	0.00000000

Table S2, Structure 9

C	-0.36331000	-3.74776700	0.00000000
C	-1.45651900	-2.82659300	0.00000000
C	-2.76198500	-3.28774400	0.00000000
C	-3.03263200	-4.70597200	0.00000000
C	-1.90702000	-5.64515600	0.00000000
C	-0.56455800	-5.11676100	0.00000000
C	-2.18488700	-7.01402400	0.00000000
C	-3.48860000	-7.52513100	0.00000000
C	-4.59579200	-6.60233300	0.00000000
C	-5.92377800	-7.14747100	0.00000000
C	-6.18940800	-8.51856800	0.00000000
C	-5.08488300	-9.43887100	0.00000000
C	-3.78462100	-8.92969600	0.00000000
C	-4.32858500	-5.22759200	0.00000000
C	-5.11477000	-10.87277500	0.00000000
C	-3.87025600	-11.42569300	0.00000000
C	-7.59419600	-8.80748200	0.00000000
C	-8.36310200	-7.68347000	0.00000000
C	0.98620300	-3.37250600	0.00000000
C	1.90574200	-4.39410400	0.00000000
C	-1.33836700	-1.42288300	0.00000000
C	-2.52744200	-0.73415300	0.00000000
S	-3.87170600	-1.89815200	0.00000000
S	1.01827300	-5.94082200	0.00000000
S	-2.60628500	-10.22697400	0.00000000
S	-7.41299200	-6.22365300	0.00000000
H	-1.34929800	-7.70985300	0.00000000
H	-5.16477600	-4.53245700	0.00000000
H	-6.02652100	-11.45956200	0.00000000
H	-8.00617500	-9.81039800	0.00000000
H	1.25396000	-2.32876900	0.00000000
H	-0.37555600	-0.93724900	0.00000000
C	7.15531700	3.77749400	0.00000000
C	5.70099800	3.69111900	0.00000000
C	5.22565700	2.39418600	0.00000000
C	6.00087200	1.20698200	0.00000000
C	7.42773400	1.24444400	0.00000000
C	7.95025700	2.59780700	0.00000000
C	8.11538900	-0.00003200	0.00000000
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C	4.59771000	4.64895300	0.00000000
C	3.34229300	4.05723700	0.00000000
S	3.51871100	2.30227800	0.00000000
S	9.65126700	3.00683800	0.00000000
S	9.65126700	-3.00690900	0.00000000
S	3.51870700	-2.30236300	0.00000000
H	9.20297400	-0.00003000	0.00000000
H	4.25567100	-0.00002500	0.00000000
H	7.54511000	-5.96401900	0.00000000
H	4.73997600	-5.72480800	0.00000000
H	7.54511700	5.96395400	0.00000000
H	4.73997300	5.72473000	0.00000000
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C	-6.18913800	8.51881100	0.00000000
C	-5.92366200	7.14769700	0.00000000
C	-4.59573600	6.60238100	0.00000000
C	-3.48847100	7.52509400	0.00000000
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C	-1.90702100	5.64506300	0.00000000
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C	-1.45651200	2.82652800	0.00000000
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C	0.98620500	3.37242800	0.00000000
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H	10.11166300	-5.42287500	0.00000000
H	-3.60817100	-12.47533700	0.00000000
H	-9.44267900	7.61610100	0.00000000
H	10.11166900	5.42280200	0.00000000
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