

Supporting Information for:

The effect of water molecules upon the hydrogen-bonding cooperativity of three-stranded antiparallel β -sheet models

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All of the optimized geometrical coordinates of the ten three-stranded antiparallel diglypeptide β -sheet models at the MP2/6-31G level.**

A:

7	0	4.836726	1.963861	0.000000
6	0	4.268024	3.186779	0.000000
8	0	4.886681	4.262120	0.000000
6	0	2.743302	3.160823	0.000000
7	0	2.274341	4.523785	0.000000
6	0	0.962553	4.815885	0.000000
8	0	0.090688	3.927034	0.000000
6	0	0.597180	6.281357	0.000000
6	0	6.274784	1.791746	0.000000
1	0	4.225606	1.152790	0.000000
1	0	2.379441	2.616764	0.871963
1	0	2.379441	2.616764	-0.871963
1	0	3.001553	5.227500	0.000000
1	0	1.466790	6.934331	0.000000
1	0	-0.008923	6.489589	-0.879194
1	0	-0.008923	6.489589	0.879194
1	0	6.600505	1.248384	0.886451
1	0	6.600505	1.248384	-0.886451
1	0	6.725063	2.779507	0.000000
7	0	0.497576	-0.643563	0.000000
6	0	1.828410	-0.849650	0.000000
8	0	2.633645	0.102661	0.000000
6	0	0.000000	0.710195	0.000000
6	0	-1.520411	0.727365	0.000000
8	0	-2.190376	-0.319108	0.000000
7	0	-2.031490	1.974074	0.000000
6	0	2.296525	-2.282480	0.000000
6	0	-3.453627	2.246796	0.000000
1	0	-0.168746	-1.409247	0.000000
1	0	0.366681	1.257711	0.870133
1	0	0.366681	1.257711	-0.870133
1	0	-1.381045	2.754396	0.000000
1	0	1.463455	-2.976969	0.000000
1	0	2.918323	-2.442606	-0.879121
1	0	2.918323	-2.442606	0.879121
1	0	-3.736538	2.813487	-0.886387
1	0	-3.736538	2.813487	0.886387
1	0	-3.982232	1.300498	0.000000
7	0	-1.009749	-5.739694	0.000000
6	0	-1.510594	-4.477441	0.000000
8	0	-0.805882	-3.460318	0.000000
6	0	-3.027279	-4.437047	0.000000
7	0	-3.517040	-3.087037	0.000000
6	0	-4.866844	-2.908008	0.000000
8	0	-5.644116	-3.870327	0.000000
6	0	-5.340942	-1.474487	0.000000
6	0	0.407438	-6.041678	0.000000
1	0	-1.664569	-6.504991	0.000000
1	0	-3.402447	-4.981102	0.872860
1	0	-3.402447	-4.981102	-0.872860

1	0	-2.862272	-2.313434	0.000000
1	0	-4.510506	-0.776428	0.000000
1	0	-5.963640	-1.316128	-0.878585
1	0	-5.963640	-1.316128	0.878585
1	0	0.683839	-6.608894	0.887769
1	0	0.683839	-6.608894	-0.887769
1	0	0.943627	-5.099797	0.000000

B:

7	0	4.655445	-1.195068	0.000000
6	0	4.914013	0.120930	0.000000
8	0	6.043437	0.648132	0.000000
6	0	3.665539	0.996620	0.000000
7	0	4.076913	2.377927	0.000000
6	0	3.175776	3.376572	0.000000
8	0	1.951160	3.155534	0.000000
6	0	3.726802	4.782791	0.000000
6	0	5.682807	-2.221551	0.000000
1	0	3.677842	-1.475398	0.000000
1	0	3.052253	0.766874	0.871631
1	0	3.052253	0.766874	-0.871631
1	0	5.075946	2.533595	0.000000
1	0	4.813895	4.811655	0.000000
1	0	3.353282	5.303379	-0.879267
1	0	3.353282	5.303379	0.879267
1	0	5.588013	-2.847682	0.886013
1	0	5.588013	-2.847682	-0.886013
1	0	6.661175	-1.756522	0.000000
8	0	8.668457	-0.518246	0.000000
1	0	9.355041	0.153307	0.000000
1	0	7.837113	-0.019724	0.000000
7	0	-0.379766	-0.784516	0.000000
6	0	0.585325	-1.723049	0.000000
8	0	1.793289	-1.411185	0.000000
6	0	0.000000	0.606865	0.000000
6	0	-1.228432	1.503011	0.000000
8	0	-2.380883	1.039399	0.000000
7	0	-0.921197	2.815278	0.000000
6	0	0.139352	-3.162554	0.000000
6	0	-1.921695	3.862222	0.000000
1	0	-1.366570	-1.022729	0.000000
1	0	0.616027	0.840056	0.870317
1	0	0.616027	0.840056	-0.870317
1	0	0.061107	3.072956	0.000000
1	0	-0.941871	-3.247547	0.000000
1	0	0.554283	-3.652473	-0.879161
1	0	0.554283	-3.652473	0.879161
1	0	-1.823924	4.487906	-0.886462
1	0	-1.823924	4.487906	0.886462
1	0	-2.900935	3.397410	0.000000
7	0	-4.557151	-4.064244	0.000000
6	0	-4.235359	-2.745039	0.000000
8	0	-3.072148	-2.322737	0.000000

6	0	-5.449337	-1.834602	0.000000
7	0	-5.067632	-0.450167	0.000000
6	0	-6.064779	0.477200	0.000000
8	0	-7.255459	0.142331	0.000000
6	0	-5.622204	1.920901	0.000000
6	0	-3.576319	-5.130851	0.000000
1	0	-5.534141	-4.309220	0.000000
1	0	-6.069816	-2.061477	0.872985
1	0	-6.069816	-2.061477	-0.872985
1	0	-4.085948	-0.198736	0.000000
1	0	-4.541058	2.010708	0.000000
1	0	-6.038756	2.410039	-0.878615
1	0	-6.038756	2.410039	0.878615
1	0	-3.679272	-5.753360	0.887772
1	0	-3.679272	-5.753360	-0.887772
1	0	-2.593825	-4.673366	0.000000

C:

7	0	4.887920	-0.509817	0.000000
6	0	4.939108	0.836278	0.000000
8	0	5.991720	1.498943	0.000000
6	0	3.567523	1.498319	0.000000
7	0	3.707027	2.933680	0.000000
6	0	2.616822	3.721594	0.000000
8	0	1.463443	3.249256	0.000000
6	0	2.873590	5.209598	0.000000
6	0	6.086961	-1.322422	0.000000
1	0	3.973955	-0.955139	0.000000
1	0	3.001303	1.160058	0.869164
1	0	3.001303	1.160058	-0.869164
1	0	4.638612	3.337234	0.000000
1	0	3.934563	5.446292	0.000000
1	0	2.400589	5.643980	-0.878682
1	0	2.400589	5.643980	0.878682
1	0	6.125212	-1.954760	0.886330
1	0	6.125212	-1.954760	-0.886330
1	0	6.941322	-0.652984	0.000000
8	0	6.420018	4.301000	0.000000
1	0	6.611302	3.712227	0.740905
1	0	6.611302	3.712227	-0.740905
7	0	-0.133320	-0.984839	0.000000
6	0	0.978555	-1.743094	0.000000
8	0	2.115540	-1.229658	0.000000
6	0	0.000000	0.451611	0.000000
6	0	-1.366170	1.119743	0.000000
8	0	-2.419770	0.460373	0.000000
7	0	-1.293908	2.464945	0.000000
6	0	0.786036	-3.238201	0.000000
6	0	-2.462570	3.319782	0.000000
1	0	-1.064281	-1.389380	0.000000
1	0	0.566938	0.788386	0.869480
1	0	0.566938	0.788386	-0.869480
1	0	-0.370965	2.891230	0.000000

1	0	-0.264535	-3.507760	0.000000
1	0	1.278837	-3.649672	-0.879227
1	0	1.278837	-3.649672	0.879227
1	0	-2.475791	3.953237	-0.886315
1	0	-2.475791	3.953237	0.886315
1	0	-3.345599	2.691150	0.000000
7	0	-3.684886	-4.941296	0.000000
6	0	-3.594001	-3.586145	0.000000
8	0	-2.520387	-2.971092	0.000000
6	0	-4.946050	-2.897403	0.000000
7	0	-4.807971	-1.468040	0.000000
6	0	-5.950060	-0.726442	0.000000
8	0	-7.065218	-1.261698	0.000000
6	0	-5.762554	0.771795	0.000000
6	0	-2.535271	-5.823183	0.000000
1	0	-4.605331	-5.350285	0.000000
1	0	-5.518376	-3.227570	0.872963
1	0	-5.518376	-3.227570	-0.872963
1	0	-3.884336	-1.050686	0.000000
1	0	-4.712855	1.045750	0.000000
1	0	-6.256979	1.182034	-0.878647
1	0	-6.256979	1.182034	0.878647
1	0	-2.529360	-6.454209	0.887770
1	0	-2.529360	-6.454209	-0.887770
1	0	-1.646221	-5.203248	0.000000

D:

7	0	3.891295	4.057455	0.000000
6	0	2.867268	4.935269	0.000000
8	0	2.985417	6.170151	0.000000
6	0	1.490310	4.280299	0.000000
7	0	0.498662	5.326343	0.000000
6	0	-0.816006	5.047508	0.000000
8	0	-1.239327	3.876512	0.000000
6	0	-1.757239	6.228431	0.000000
6	0	5.271714	4.495854	0.000000
1	0	3.670749	3.066373	0.000000
1	0	1.384323	3.634322	0.871929
1	0	1.384323	3.634322	-0.871929
1	0	0.868514	6.268273	0.000000
1	0	-1.237642	7.183741	0.000000
1	0	-2.395117	6.166009	-0.879156
1	0	-2.395117	6.166009	0.879156
1	0	5.793056	4.136053	0.886479
1	0	5.793056	4.136053	-0.886479
1	0	5.272724	5.581398	0.000000
7	0	1.012408	-0.112246	0.000000
6	0	2.310050	0.248252	0.000000
8	0	2.652210	1.447269	0.000000
6	0	0.000000	0.914986	0.000000
6	0	-1.391465	0.301596	0.000000
8	0	-1.567864	-0.929085	0.000000
7	0	-2.371937	1.224507	0.000000

6	0	3.326220	-0.865280	0.000000
6	0	-3.780801	0.887949	0.000000
1	0	0.720523	-1.084079	0.000000
1	0	0.107588	1.565121	0.870075
1	0	0.107588	1.565121	-0.870075
1	0	-2.101480	2.203782	0.000000
1	0	2.852522	-1.840965	0.000000
1	0	3.958873	-0.755849	-0.879118
1	0	3.958873	-0.755849	0.879118
1	0	-4.271069	1.288503	-0.886421
1	0	-4.271069	1.288503	0.886421
1	0	-3.874920	-0.191607	0.000000
7	0	1.720050	-5.378557	0.000000
6	0	0.747254	-4.432141	0.000000
8	0	0.971144	-3.215532	0.000000
6	0	-0.653980	-5.015213	0.000000
7	0	-1.651081	-3.979075	0.000000
6	0	-2.952043	-4.353011	0.000000
8	0	-3.262885	-5.559825	0.000000
6	0	-3.976211	-3.250089	0.000000
6	0	3.137069	-5.073226	0.000000
1	0	1.436943	-6.345200	0.000000
1	0	-0.777570	-5.662783	0.873497
1	0	-0.777570	-5.662783	-0.873497
1	0	-1.367369	-3.004684	0.000000
1	0	-3.504212	-2.274076	0.000000
1	0	-4.613787	-3.368979	-0.873592
1	0	-4.613787	-3.368979	0.873592
1	0	3.620844	-5.477738	0.887870
1	0	3.620844	-5.477738	-0.887870
1	0	3.240419	-3.994381	0.000000
8	0	-6.116628	-5.600478	0.000000
1	0	-5.149790	-5.703108	0.000000
1	0	-6.446413	-6.502974	0.000000

E:

7	0	-4.207260	3.527731	0.000000
6	0	-5.073356	2.494091	0.000000
8	0	-6.309739	2.598145	0.000000
6	0	-4.403285	1.124151	0.000000
7	0	-5.439176	0.121802	0.000000
6	0	-5.148448	-1.190237	0.000000
8	0	-3.974388	-1.604510	0.000000
6	0	-6.321809	-2.141393	0.000000
6	0	-4.661447	4.902944	0.000000
1	0	-3.213375	3.318206	0.000000
1	0	-3.756195	1.025221	0.871854
1	0	-3.756195	1.025221	-0.871854
1	0	-6.384615	0.482664	0.000000
1	0	-7.281398	-1.629720	0.000000
1	0	-6.254037	-2.778672	-0.879203
1	0	-6.254037	-2.778672	0.879203
1	0	-4.307448	5.428403	0.886411

1	0	-4.307448	5.428403	-0.886411
1	0	-5.746956	4.891836	0.000000
7	0	0.000000	0.713552	0.000000
6	0	-0.386216	2.003858	0.000000
8	0	-1.593178	2.319579	0.000000
6	0	-1.012103	-0.314051	0.000000
6	0	-0.385546	-1.699065	0.000000
8	0	0.845366	-1.867737	0.000000
7	0	-1.300674	-2.688552	0.000000
6	0	0.704513	3.043786	0.000000
6	0	-0.947193	-4.092602	0.000000
1	0	0.978953	0.443265	0.000000
1	0	-1.664107	-0.214836	0.869880
1	0	-1.664107	-0.214836	-0.869880
1	0	-2.282695	-2.428742	0.000000
1	0	1.690358	2.591688	0.000000
1	0	0.580052	3.673933	-0.879015
1	0	0.580052	3.673933	0.879015
1	0	-1.341157	-4.588697	-0.886359
1	0	-1.341157	-4.588697	0.886359
1	0	0.133947	-4.171568	0.000000
7	0	5.236326	1.525104	0.000000
6	0	4.296192	0.553790	0.000000
8	0	3.072142	0.755974	0.000000
6	0	4.896809	-0.840792	0.000000
7	0	3.891456	-1.864621	0.000000
6	0	4.322394	-3.153766	0.000000
8	0	5.531015	-3.428333	0.000000
6	0	3.246439	-4.212456	0.000000
6	0	4.918081	2.937669	0.000000
1	0	6.209125	1.235141	0.000000
1	0	5.548653	-0.949256	0.870842
1	0	5.548653	-0.949256	-0.870842
1	0	2.909592	-1.611939	0.000000
1	0	2.253743	-3.774738	0.000000
1	0	3.378730	-4.841297	-0.878567
1	0	3.378730	-4.841297	0.878567
1	0	5.321913	3.425534	0.886444
1	0	5.321913	3.425534	-0.886444
1	0	3.838708	3.039722	0.000000
8	0	7.962571	0.241146	0.000000
1	0	8.038316	-0.350627	0.757174
1	0	8.038316	-0.350627	-0.757174

F:

7	0	-5.052244	0.517632	0.000000
6	0	-5.181941	-0.817022	0.000000
8	0	-6.255122	-1.451418	0.000000
6	0	-3.854722	-1.567949	0.000000
7	0	-4.130899	-2.982631	0.000000
6	0	-3.137599	-3.889484	0.000000
8	0	-1.939948	-3.551508	0.000000
6	0	-3.550268	-5.342342	0.000000

6	0	-6.174098	1.439946	0.000000
1	0	-4.106241	0.891506	0.000000
1	0	-3.266141	-1.280150	0.871379
1	0	-3.266141	-1.280150	-0.871379
1	0	-5.110343	-3.233631	0.000000
1	0	-4.629502	-5.476137	0.000000
1	0	-3.128267	-5.824515	-0.879249
1	0	-3.128267	-5.824515	0.879249
1	0	-6.140041	2.072320	0.885978
1	0	-6.140041	2.072320	-0.885978
1	0	-7.103024	0.882702	0.000000
8	0	-8.980608	-0.544919	0.000000
1	0	-9.596291	-1.282097	0.000000
1	0	-8.103783	-0.958537	0.000000
7	0	0.000000	0.603659	0.000000
6	0	-1.057249	1.437227	0.000000
8	0	-2.226134	0.999624	0.000000
6	0	-0.239161	-0.818725	0.000000
6	0	1.068378	-1.593927	0.000000
8	0	2.173205	-1.026268	0.000000
7	0	0.886305	-2.929679	0.000000
6	0	-0.764927	2.915189	0.000000
6	0	1.981624	-3.876750	0.000000
1	0	0.956657	0.945055	0.000000
1	0	-0.830100	-1.111315	0.869936
1	0	-0.830100	-1.111315	-0.869936
1	0	-0.066897	-3.279785	0.000000
1	0	0.301394	3.113147	0.000000
1	0	-1.229648	3.358544	-0.879033
1	0	-1.229648	3.358544	0.879033
1	0	1.943964	-4.508986	-0.886441
1	0	1.943964	-4.508986	0.886441
1	0	2.912119	-3.320599	0.000000
7	0	3.813814	4.275143	0.000000
6	0	3.603662	2.939962	0.000000
8	0	2.486006	2.401035	0.000000
6	0	4.897294	2.144765	0.000000
7	0	4.663930	0.728922	0.000000
6	0	5.757967	-0.077847	0.000000
8	0	6.904495	0.392681	0.000000
6	0	5.487137	-1.562897	0.000000
6	0	2.741188	5.247887	0.000000
1	0	4.776372	4.597599	0.000000
1	0	5.492779	2.431099	0.870851
1	0	5.492779	2.431099	-0.870851
1	0	3.715440	0.371102	0.000000
1	0	4.423466	-1.776631	0.000000
1	0	5.957292	-2.000932	-0.878574
1	0	5.957292	-2.000932	0.878574
1	0	2.791160	5.879189	0.886451
1	0	2.791160	5.879189	-0.886451
1	0	1.799332	4.710956	0.000000
8	0	6.781490	4.794749	0.000000
1	0	7.186089	4.356758	0.757369
1	0	7.186089	4.356758	-0.757369

G:

7	0	4.215553	3.231823	0.000000
6	0	3.325624	4.243115	0.000000
8	0	3.632708	5.448408	0.000000
6	0	1.875318	3.778882	0.000000
7	0	0.988310	4.915936	0.000000
6	0	-0.344742	4.736269	0.000000
8	0	-0.854703	3.598928	0.000000
6	0	-1.183843	5.991377	0.000000
6	0	5.644686	3.467983	0.000000
1	0	3.859545	2.279802	0.000000
1	0	1.697297	3.143666	0.869098
1	0	1.697297	3.143666	-0.869098
1	0	1.386326	5.849797	0.000000
1	0	-0.578037	6.893985	0.000000
1	0	-1.826000	5.980427	-0.878625
1	0	-1.826000	5.980427	0.878625
1	0	6.107704	3.035785	0.886362
1	0	6.107704	3.035785	-0.886362
1	0	5.803179	4.541714	0.000000
8	0	2.014349	7.778056	0.000000
1	0	2.557251	7.480157	0.740801
1	0	2.557251	7.480157	-0.740801
7	0	0.891137	-0.568183	0.000000
6	0	2.220084	-0.355286	0.000000
8	0	2.693977	0.798508	0.000000
6	0	0.000000	0.566292	0.000000
6	0	-1.451142	0.111073	0.000000
8	0	-1.761642	-1.093178	0.000000
7	0	-2.323804	1.136152	0.000000
6	0	3.106762	-1.574498	0.000000
6	0	-3.760985	0.956102	0.000000
1	0	0.492217	-1.501250	0.000000
1	0	0.179956	1.200773	0.869376
1	0	0.179956	1.200773	-0.869376
1	0	-1.946342	2.080111	0.000000
1	0	2.528073	-2.491819	0.000000
1	0	3.747563	-1.535696	-0.879203
1	0	3.747563	-1.535696	0.879203
1	0	-4.204428	1.408191	-0.886347
1	0	-4.204428	1.408191	0.886347
1	0	-3.973516	-0.106500	0.000000
7	0	1.009670	-5.882071	0.000000
6	0	0.149080	-4.832366	0.000000
8	0	0.508051	-3.648607	0.000000
6	0	-1.308669	-5.254874	0.000000
7	0	-2.183866	-4.113980	0.000000
6	0	-3.518439	-4.341035	0.000000
8	0	-3.961173	-5.505902	0.000000
6	0	-4.413833	-3.131160	0.000000
6	0	2.451884	-5.737322	0.000000
1	0	0.619790	-6.810802	0.000000

1	0	-1.503564	-5.884600	0.873545
1	0	-1.503564	-5.884600	-0.873545
1	0	-1.793628	-3.177104	0.000000
1	0	-3.836494	-2.213523	0.000000
1	0	-5.060583	-3.178683	-0.873651
1	0	-5.060583	-3.178683	0.873651
1	0	2.887488	-6.193373	0.887868
1	0	2.887488	-6.193373	-0.887868
1	0	2.675300	-4.676794	0.000000
8	0	-6.802596	-5.230723	0.000000
1	0	-5.852994	-5.438809	0.000000
1	0	-7.230276	-6.091069	0.000000

H:

7	0	2.964302	-3.426260	0.000000
6	0	3.908034	-2.475971	0.000000
8	0	5.141548	-2.680649	0.000000
6	0	3.347055	-1.060043	0.000000
7	0	4.415139	-0.091302	0.000000
6	0	4.134304	1.225460	0.000000
8	0	2.961861	1.646288	0.000000
6	0	5.322228	2.157207	0.000000
6	0	3.243929	-4.851494	0.000000
1	0	1.993694	-3.118332	0.000000
1	0	2.700375	-0.928356	0.868794
1	0	2.700375	-0.928356	-0.868794
1	0	5.376126	-0.414673	0.000000
1	0	6.268546	1.622234	0.000000
1	0	5.262472	2.796531	-0.878685
1	0	5.262472	2.796531	0.878685
1	0	2.814537	-5.316749	0.885924
1	0	2.814537	-5.316749	-0.885924
1	0	4.314583	-5.013894	0.000000
8	0	6.683957	-5.112439	0.000000
1	0	7.624092	-4.915445	0.000000
1	0	6.244158	-4.249199	0.000000
8	0	7.358588	-0.900588	0.000000
1	0	7.082482	-1.450070	0.744032
1	0	7.082482	-1.450070	-0.744032
7	0	-1.061086	-0.405175	0.000000
6	0	-0.741818	-1.711938	0.000000
8	0	0.448130	-2.088756	0.000000
6	0	0.000000	0.572238	0.000000
6	0	-0.565951	1.983596	0.000000
8	0	-1.789490	2.200523	0.000000
7	0	0.389558	2.933512	0.000000
6	0	-1.882848	-2.696205	0.000000
6	0	0.095272	4.351409	0.000000
1	0	-2.023875	-0.083039	0.000000
1	0	0.646332	0.442035	0.869553
1	0	0.646332	0.442035	-0.869553
1	0	1.359735	2.631045	0.000000
1	0	-2.844652	-2.195019	0.000000

1	0	-1.790847	-3.331583	-0.879204
1	0	-1.790847	-3.331583	0.879204
1	0	0.509848	4.830297	-0.886388
1	0	0.509848	4.830297	0.886388
1	0	-0.981445	4.476321	0.000000
7	0	-6.341600	-0.969551	0.000000
6	0	-5.367998	-0.022933	0.000000
8	0	-4.158246	-0.283550	0.000000
6	0	-5.912854	1.393214	0.000000
7	0	-4.854652	2.364012	0.000000
6	0	-5.208320	3.679062	0.000000
8	0	-6.395471	4.026370	0.000000
6	0	-4.067559	4.668285	0.000000
6	0	-6.077512	-2.394263	0.000000
1	0	-7.299426	-0.657941	0.000000
1	0	-6.559219	1.530398	0.872927
1	0	-6.559219	1.530398	-0.872927
1	0	-3.888881	2.056880	0.000000
1	0	-3.103429	4.170919	0.000000
1	0	-4.161244	5.303910	-0.878607
1	0	-4.161244	5.303910	0.878607
1	0	-6.495512	-2.866942	0.887766
1	0	-6.495512	-2.866942	-0.887766
1	0	-5.002094	-2.528781	0.000000

I:

7	0	-3.396923	4.775508	0.000000
6	0	-4.487757	3.982337	0.000000
8	0	-5.661934	4.382940	0.000000
6	0	-4.169324	2.490964	0.000000
7	0	-5.416765	1.768826	0.000000
6	0	-5.451029	0.425306	0.000000
8	0	-4.411106	-0.259225	0.000000
6	0	-6.818919	-0.215169	0.000000
6	0	-3.504474	6.219776	0.000000
1	0	-2.483565	4.331531	0.000000
1	0	-3.565400	2.238465	0.871896
1	0	-3.565400	2.238465	-0.871896
1	0	-6.247238	2.347035	0.000000
1	0	-7.626884	0.512701	0.000000
1	0	-6.906619	-0.849999	-0.879209
1	0	-6.906619	-0.849999	0.879209
1	0	-3.033859	6.643936	0.886440
1	0	-3.033859	6.643936	-0.886440
1	0	-4.560384	6.471801	0.000000
7	0	0.000000	1.018557	0.000000
6	0	-0.058512	2.364206	0.000000
8	0	-1.150693	2.966578	0.000000
6	0	-1.231617	0.268088	0.000000
6	0	-0.958804	-1.227649	0.000000
8	0	0.195758	-1.688148	0.000000
7	0	-2.085367	-1.966135	0.000000
6	0	1.254448	3.104399	0.000000

6	0	-2.085144	-3.414412	0.000000
1	0	0.882552	0.516694	0.000000
1	0	-1.839947	0.522380	0.869939
1	0	-1.839947	0.522380	-0.869939
1	0	-2.974915	-1.475532	0.000000
1	0	2.099039	2.423962	0.000000
1	0	1.288909	3.745692	-0.879065
1	0	1.288909	3.745692	0.879065
1	0	-2.588415	-3.798749	-0.886398
1	0	-2.588415	-3.798749	0.886398
1	0	-1.056701	-3.756233	0.000000
7	0	5.273822	0.513077	0.000000
6	0	4.126310	-0.199949	0.000000
8	0	2.987442	0.291344	0.000000
6	0	4.367476	-1.700141	0.000000
7	0	3.135692	-2.440408	0.000000
6	0	3.215822	-3.789431	0.000000
8	0	4.327809	-4.357341	0.000000
6	0	1.917769	-4.551118	0.000000
6	0	5.307473	1.961077	0.000000
1	0	6.147790	-0.003217	0.000000
1	0	4.969710	-1.968330	0.871505
1	0	4.969710	-1.968330	-0.871505
1	0	2.248034	-1.947774	0.000000
1	0	1.067139	-3.878852	0.000000
1	0	1.895447	-5.199245	-0.873687
1	0	1.895447	-5.199245	0.873687
1	0	5.817705	2.335808	0.886518
1	0	5.817705	2.335808	-0.886518
1	0	4.285227	2.322093	0.000000
8	0	3.747961	-7.151377	0.000000
1	0	4.051301	-6.227562	0.000000
1	0	4.559597	-7.665419	0.000000
8	0	7.619249	-1.359738	0.000000
1	0	7.591263	-1.953549	0.758520
1	0	7.591263	-1.953549	-0.758520

J:

7	0	4.882013	1.668341	0.000000
6	0	4.419203	2.924976	0.000000
8	0	5.125834	3.956719	0.000000
6	0	2.898967	3.015421	0.000000
7	0	2.473508	4.393232	0.000000
6	0	1.161736	4.696526	0.000000
8	0	0.284115	3.812555	0.000000
6	0	0.820819	6.167243	0.000000
6	0	6.291993	1.319719	0.000000
1	0	4.193010	0.918491	0.000000
1	0	2.505786	2.485177	0.868631
1	0	2.505786	2.485177	-0.868631
1	0	3.173560	5.126441	0.000000
1	0	1.706228	6.797970	0.000000
1	0	0.216356	6.383965	-0.878656

1	0	0.216356	6.383965	0.878656
1	0	6.532136	0.733909	0.885909
1	0	6.532136	0.733909	-0.885909
1	0	6.891680	2.221413	0.000000
8	0	7.981568	4.328715	0.000000
1	0	7.013349	4.293621	0.000000
1	0	8.198189	5.264574	0.000000
8	0	4.458554	6.719798	0.000000
1	0	4.833961	6.232280	0.743753
1	0	4.833961	6.232280	-0.743753
7	0	0.439510	-0.703346	0.000000
6	0	1.759921	-0.961190	0.000000
8	0	2.599916	-0.037584	0.000000
6	0	0.000000	0.670700	0.000000
6	0	-1.517882	0.757282	0.000000
8	0	-2.235818	-0.257545	0.000000
7	0	-1.971611	2.025458	0.000000
6	0	2.175950	-2.409274	0.000000
6	0	-3.379848	2.364091	0.000000
1	0	-0.255283	-1.444008	0.000000
1	0	0.391318	1.201982	0.869258
1	0	0.391318	1.201982	-0.869258
1	0	-1.285230	2.774838	0.000000
1	0	1.317927	-3.072638	0.000000
1	0	2.791698	-2.591557	-0.879122
1	0	2.791698	-2.591557	0.879122
1	0	-3.635749	2.943308	-0.886400
1	0	-3.635749	2.943308	0.886400
1	0	-3.952897	1.444223	0.000000
7	0	-1.280944	-5.708940	0.000000
6	0	-1.705460	-4.426522	0.000000
8	0	-0.960986	-3.434241	0.000000
6	0	-3.220422	-4.310252	0.000000
7	0	-3.653014	-2.939810	0.000000
6	0	-4.983711	-2.703420	0.000000
8	0	-5.794851	-3.652578	0.000000
6	0	-5.422100	-1.263651	0.000000
6	0	0.118726	-6.081420	0.000000
1	0	-1.987700	-6.437640	0.000000
1	0	-3.621748	-4.833374	0.871446
1	0	-3.621748	-4.833374	-0.871446
1	0	-2.967360	-2.191245	0.000000
1	0	-4.570276	-0.592903	0.000000
1	0	-6.047258	-1.091008	-0.873641
1	0	-6.047258	-1.091008	0.873641
1	0	0.363194	-6.665360	0.886508
1	0	0.363194	-6.665360	-0.886508
1	0	0.709670	-5.172554	0.000000
8	0	-8.375896	-2.434661	0.000000
1	0	-7.549692	-2.947240	0.000000
1	0	-9.066994	-3.102020	0.000000
8	0	-3.647725	-7.552062	0.000000
1	0	-4.219419	-7.389410	0.758580
1	0	-4.219419	-7.389410	-0.758580