Supporting Information part II for:

Improved Polarizable Dipole–Dipole Interaction Model for Hydrogen Bonding, Stacking, T-Shaped and X–H···π Interactions

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Table S23. Cartesian x, y, z coordinates in angstroms for the 19 training dimers.

U···U (BP)

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.729999	0.022768	0.000915
C	-1.296825	-1.240427	0.001502
O	-0.594099	-2.253518	0.002634
C	-2.743622	-1.262332	0.000479
C	-3.422020	-0.095909	-0.000923
N	-2.774837	1.105409	-0.001418
C	-1.391479	1.237020	-0.000525
O	-0.839844	2.317035	-0.001001
H	0.298423	0.074004	0.001623
H	-3.249590	-2.211835	0.000833
H	-4.500897	-0.049216	-0.001745
H	-3.283838	1.973877	-0.002486
N	4.143829	-1.085704	0.000499
C	4.999877	-2.200322	-0.001001
O	6.209329	-2.048617	-0.001750
C	4.285659	-3.462495	-0.001505
C	2.935490	-3.466313	-0.000545
N	2.197498	-2.315432	0.000906
C	2.770269	-1.070767	0.001456
O	2.119948	-0.029549	0.002693
H	4.591073	-0.179131	0.000886
H	4.852243	-4.377526	-0.002644
H	2.358527	-4.379278	-0.000864
H	1.171162	-2.336875	0.001583

water···water

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.702196	-0.056060	0.009942
H	-1.022193	0.846776	-0.011489
H	0.257521	0.042121	0.005219
O	2.220871	0.026717	0.000620
H	2.597493	-0.411663	0.766745
H	2.593135	-0.449496	-0.744782

MeOH···$MeNH_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.706920	0.045830	0.006386

C	-1.076671	-1.313916	0.001614
H	0.265624	0.071710	0.001339
H	-2.162924	-1.363196	0.005865
H	-0.723406	-1.844652	-0.887743
H	-0.716080	-1.852821	0.883080
N	2.201272	-0.036421	-0.003338
C	2.679024	-1.422454	0.034123
H	2.571892	0.471356	0.789794
H	2.572015	0.427918	-0.822597
H	2.287140	-1.956480	-0.828069
H	3.765736	-1.529189	0.037157
H	2.286898	-1.909184	0.923755

$MeNH_2 \cdots MeOH$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.893451	-0.043844	-0.042997
C	-1.175782	0.757908	1.145237
H	0.096948	-0.256059	-0.071070
H	-1.368439	-0.933391	0.033838
H	-2.241627	0.972216	1.195025
H	-0.880790	0.304247	2.097209
H	-0.663006	1.714329	1.060809
O	2.284460	-0.047476	0.027825
C	2.670373	0.864108	1.047261
H	2.566486	0.322472	-0.812039
H	2.347190	0.434475	1.990328
H	3.751429	1.003191	1.086301
H	2.191899	1.837706	0.932085

$MeNH_2 \cdots MeNH_2$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.638641	0.470916	0.044568
C	-1.198659	0.391399	1.391947
H	0.189954	-0.113937	-0.005774
H	-1.300469	0.081257	-0.613668
H	-2.092738	1.009245	1.453167
H	-1.462746	-0.615844	1.729452
H	-0.480276	0.798675	2.101087
N	2.398893	-0.455521	0.197045
C	2.559123	0.679689	1.110720
H	2.695162	-0.180983	-0.730941

H	3.022443	-1.203211	0.472239
H	2.288933	0.364994	2.116373
H	3.566534	1.101466	1.147692
H	1.866583	1.465465	0.818063

water···pyridine

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	-0.552831	-0.101697	-0.000499
H	-0.871760	0.801792	0.000144
H	0.412659	-0.001832	-0.000252
N	2.364021	0.096623	0.000147
C	3.059928	0.062652	1.144895
C	4.448951	-0.002531	1.194891
C	5.160114	-0.035656	-0.000020
C	4.448806	-0.002597	-1.194822
C	3.059776	0.062598	-1.144675
H	2.475255	0.086263	2.055763
H	4.954858	-0.027385	2.149220
H	6.239954	-0.087430	-0.000101
H	4.954603	-0.027470	-2.149220
H	2.475007	0.086198	-2.055468

AcOH···AcOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.061709	1.297141	0.292060
O	-0.358161	2.270459	0.531813
O	-0.589304	0.094918	0.003789
C	-2.558428	1.342550	0.296257
H	0.404436	0.127723	0.018412
H	-2.895998	2.347464	0.518316
H	-2.932889	1.022390	-0.672996
H	-2.937212	0.644910	1.039557
C	2.789348	1.108419	0.271184
O	2.085730	0.135105	0.031396
O	2.316922	2.310855	0.558962
C	4.286061	1.062516	0.269219
H	1.323134	2.277956	0.544562
H	4.623640	0.061197	0.031694
H	4.667559	1.772869	-0.460250
H	4.657577	1.365211	1.245275

$AcNH_2\cdots AcNH_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.309750	1.180176	-0.025170
O	-0.725300	2.155148	0.452713
N	-0.665621	0.095055	-0.491994
C	-2.816719	1.155999	-0.110606
H	0.354583	0.051448	-0.459309
H	-1.183627	-0.673600	-0.870756
H	-3.220629	1.262541	0.893082
H	-3.209428	0.248634	-0.561900
H	-3.143158	2.016596	-0.688893
C	2.779602	1.063886	0.134357
O	2.195180	0.089865	-0.345374
N	2.135514	2.148629	0.602204
C	4.286601	1.088170	0.219582
H	1.115409	2.193067	0.567902
H	2.653538	2.916590	0.982324
H	4.678472	1.987820	0.686766
H	4.690157	1.000625	-0.786198
H	4.614380	0.217595	0.781763

PHE PHE st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.712645	1.120996	0.060541
C	1.258236	-0.159252	0.124234
C	0.426885	-1.274527	0.042650
C	-0.949578	-1.110074	-0.100314
C	-1.495526	0.171051	-0.161546
C	-0.663828	1.286643	-0.083401
H	1.357842	1.986399	0.127737
H	2.324954	-0.287100	0.246743
H	0.850445	-2.268433	0.094750
H	-1.594456	-1.976274	-0.163713
H	-2.563783	0.299221	-0.273703
H	-1.086901	2.281000	-0.132886
C	1.987760	1.109757	3.710320
C	2.533714	-0.171394	3.771839
C	1.702064	-1.286994	3.693189
C	0.325663	-1.121359	3.548472
C	-0.219897	0.158874	3.484506
C	0.611380	1.274155	3.566577
H	2.632606	1.975941	3.774070

H	3.601920	-0.299541	3.884584
H	2.125146	-2.281346	3.742843
H	-0.319440	-1.986769	3.480840
H	-1.286525	0.286703	3.361328
H	0.187855	2.268060	3.514208

PHE pyridine st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.818747	0.864172	0.188286
C	1.368997	-0.390524	-0.066698
C	0.534379	-1.488493	-0.271888
C	-0.849116	-1.330507	-0.219896
C	-1.399485	-0.076030	0.040434
C	-0.565292	1.021403	0.242279
H	1.466114	1.716668	0.344721
H	2.443036	-0.511862	-0.110574
H	0.960848	-2.461564	-0.475507
H	-1.497069	-2.181860	-0.379553
H	-2.472687	0.044908	0.093382
H	-0.992557	1.993661	0.446258
N	-2.398432	0.162141	3.520411
C	-1.783546	1.319809	3.800476
C	-0.401331	1.460656	3.890646
C	0.399620	0.343677	3.676432
C	-0.220932	-0.864978	3.382773
C	-1.611446	-0.903016	3.317323
H	-2.431150	2.172980	3.962988
H	0.030518	2.424307	4.121863
H	1.477189	0.414061	3.731267
H	0.354843	-1.760600	3.198698
H	-2.120299	-1.831469	3.088481

U U st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	1.376901	0.839747	0.734625
C	1.308983	1.457530	-0.520655
O	0.920561	2.611078	-0.625977
N	2.011423	-1.213208	-0.098072
C	2.025737	-0.697171	-1.364397
C	1.714512	0.591938	-1.612487
C	1.645945	-0.485206	1.018718

O	1.561116	-0.971816	2.129809
H	1.051812	1.386224	1.523356
H	2.129454	-2.201521	0.056829
H	2.297517	-1.391060	-2.145645
H	1.727286	0.990843	-2.611996
N	-1.355461	-0.836046	0.734625
C	-1.287542	-1.453828	-0.520655
O	-0.899121	-2.607376	-0.625977
N	-1.989983	1.216910	-0.098072
C	-2.004297	0.700873	-1.364397
C	-1.693072	-0.588236	-1.612487
C	-1.624505	0.488908	1.018718
O	-1.539676	0.975518	2.129809
H	-1.030372	-1.382522	1.523356
H	-2.108014	2.205222	0.056829
H	-2.276077	1.394762	-2.145645
H	-1.705845	-0.987141	-2.611996

PHE PHE TS

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.729189	1.113101	0.326728
C	1.375087	-0.119366	0.412777
C	0.635040	-1.280553	0.629385
C	-0.750986	-1.209654	0.757890
C	-1.397034	0.022671	0.673090
C	-0.656897	1.184296	0.458339
H	1.303216	2.014222	0.159160
H	2.450515	-0.174624	0.313307
H	1.136334	-2.236017	0.700217
H	-1.324526	-2.111413	0.924199
H	-2.472425	0.078488	0.773998
H	-1.157828	2.140587	0.395096
C	0.158106	0.152890	4.085883
C	-0.932975	-0.602008	4.513219
C	-1.093675	-0.896134	5.866169
C	-0.161793	-0.435080	6.794663
C	0.929792	0.320022	6.369423
C	1.088596	0.613507	5.015932
H	0.280233	0.378374	3.035456
H	-1.653480	-0.958523	3.789525
H	-1.940783	-1.482102	6.196417
H	-0.285686	-0.663046	7.844671
H	1.652911	0.677855	7.089806
H	1.935854	1.199582	4.685884

PHE pyridine TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.845077	1.057919	0.699455
C	1.375509	-0.217455	0.511161
C	0.524068	-1.307044	0.333192
C	-0.857716	-1.121463	0.346384
C	-1.388046	0.153634	0.537613
C	-0.536613	1.243422	0.712739
H	1.506406	1.903222	0.833382
H	2.447184	-0.361473	0.502852
H	0.935727	-2.296026	0.184923
H	-1.518381	-1.966458	0.208363
H	-2.459718	0.297416	0.550032
H	-0.948924	2.232806	0.857366
N	0.023117	0.352025	6.774545
C	0.177801	1.289986	5.829668
C	0.163592	1.022696	4.463168
C	-0.020746	-0.288933	4.037878
C	-0.182595	-1.273968	5.006737
C	-0.153393	-0.906635	6.349826
H	0.319572	2.302512	6.187569
H	0.293832	1.823722	3.749283
H	-0.037313	-0.532052	2.984530
H	-0.329138	-2.309179	4.731965
H	-0.276989	-1.654148	7.123927

pyridine pyridine TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.322763	-0.010376	1.019184
C	0.651286	-1.148992	0.796801
C	-0.672681	-1.194712	0.366657
C	-1.347197	0.003134	0.152144
C	-0.664558	1.194091	0.379002
C	0.658896	1.134979	0.808860
H	1.200418	-2.065528	0.973673
H	-1.157194	-2.147321	0.206464
H	-2.375357	0.008405	-0.182293
H	-1.142626	2.151558	0.228721
H	1.214103	2.045910	0.995438
N	0.450115	0.001301	6.780960
C	1.320783	-0.004312	5.761547

C	0.947397	-0.011380	4.419719
C	-0.408651	-0.012794	4.107303
C	-1.326754	-0.007078	5.152473
C	-0.851151	-0.000161	6.461432
H	2.368640	-0.003063	6.035849
H	1.694858	-0.015544	3.638619
H	-0.738380	-0.018249	3.077022
H	-2.391205	-0.007928	4.963737
H	-1.543334	0.004422	7.294623

PHE···water (OH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.780147	-0.609915	-1.207557
C	0.477943	0.750994	-1.207895
C	0.327289	1.431868	-0.000000
C	0.477943	0.750994	1.207895
C	0.780147	-0.609915	1.207557
C	0.931648	-1.289981	0.000000
H	0.896192	-1.137640	-2.144145
H	0.356964	1.278168	-2.144054
H	0.091465	2.487139	0.000000
H	0.356964	1.278168	2.144054
H	0.896192	-1.137640	2.144145
H	1.168486	-2.345214	-0.000000
O	-2.743831	-0.269263	0.000000
H	-2.579027	-1.213984	0.000000
H	-1.856530	0.102328	0.000000

PHE···$MeNH_2$ (NH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.692315	1.088292	0.324841
C	1.318187	-0.156870	0.286896
C	0.558018	-1.321950	0.381400
C	-0.827552	-1.241422	0.511685
C	-1.453411	0.003671	0.548381
C	-0.693461	1.168401	0.456229
H	1.281949	1.991947	0.252516
H	2.393143	-0.219476	0.188407
H	1.043919	-2.287574	0.357615
H	-1.416701	-2.145252	0.585339
H	-2.528233	0.065703	0.649843

H	-1.178735	2.134410	0.485727
N	0.275065	-0.222717	3.858907
C	-1.101035	-0.629101	4.136343
H	0.409683	-0.178677	2.855836
H	0.416557	0.722429	4.191379
H	-1.258911	-0.657648	5.212898
H	-1.872337	0.011280	3.696224
H	-1.255727	-1.638668	3.760721

U···ethyne

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.055454	-0.947991	0.010010
C	-1.313960	-0.335145	-0.064586
O	-2.328897	-1.007901	-0.123103
C	-1.248359	1.116052	-0.066509
C	-0.053080	1.731427	0.034195
N	1.115926	1.027591	0.135169
C	1.175347	-0.353805	0.176166
O	2.214631	-0.966465	0.335172
H	-0.057316	-1.957713	0.055053
H	-2.164349	1.675333	-0.147102
H	0.048111	2.806430	0.043420
H	1.996655	1.497280	0.261620
C	0.707852	-0.172302	3.276351
C	-0.436752	0.214155	3.382543
H	1.703670	-0.526288	3.162133
H	-1.441635	0.542856	3.482907

pyridine···ethene

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	1.381382	-0.000233	0.131464
C	0.679351	-1.140239	0.092080
C	-0.709722	-1.193114	0.006664
C	-1.421614	0.000133	-0.040817
C	-0.709401	1.193175	0.006522
C	0.679652	1.139956	0.091893
H	1.258720	-2.054962	0.125884
H	-1.214088	-2.148562	-0.025309
H	-2.500696	0.000258	-0.109170
H	-1.213512	2.148748	-0.025528

H	1.259261	2.054511	0.125502
C	0.019605	0.666439	3.487272
C	0.019937	-0.666248	3.487405
H	0.930079	1.225925	3.328157
H	-0.889943	1.228844	3.644233
H	0.930673	-1.225330	3.328394
H	-0.889351	-1.229073	3.644494

neopentane···pentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.530383	-0.417575	0.681306
C	-1.276157	0.443635	0.750025
C	0.002205	-0.380716	0.678993
C	1.268333	0.462396	0.749369
C	2.534966	-0.380425	0.680686
H	-2.559886	-0.982790	-0.250156
H	-2.554036	-1.133865	1.502658
H	-3.436214	0.184144	0.736771
H	-1.278084	1.025218	1.675085
H	-1.280339	1.168556	-0.067158
H	0.007829	-1.111413	1.493831
H	0.006249	-0.960523	-0.248820
H	1.262020	1.044250	1.674246
H	1.261635	1.187057	-0.068035
H	2.572440	-0.945717	-0.250452
H	3.431981	0.234415	0.735578
H	2.569208	-1.095810	1.502456
C	-0.000521	0.063971	5.241306
C	0.000551	-0.076160	6.761039
C	-1.239977	-0.617681	4.667408
C	1.252084	-0.593570	4.667836
C	-0.014769	1.543764	4.866685
H	-0.886485	0.387916	7.194409
H	0.009802	-1.126940	7.054049
H	0.879211	0.403505	7.194682
H	-1.263276	-0.528724	3.580579
H	-1.252062	-1.678957	4.920421
H	-2.150920	-0.165389	5.062493
H	1.273411	-0.505284	3.580865
H	1.285214	-1.654130	4.921928
H	2.153896	-0.122926	5.062257
H	0.862997	2.054351	5.265640
H	-0.015293	1.670219	3.783033
H	-0.902875	2.037097	5.264473

Table S24. Cartesian x, y, z coordinates in angstroms for the 124 small testing dimers.

1 U···U (C_{2h})

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.427109	1.066759	0.000000
C	-0.555493	1.936599	0.000000
N	0.783678	1.659890	0.000000
C	1.737608	2.641613	0.000000
C	1.427109	3.955160	0.000000
C	0.036033	4.363901	0.000000
N	-0.854827	3.274218	0.000000
O	-0.389849	5.505030	0.000000
H	1.049161	0.667082	0.000000
H	2.757251	2.285964	0.000000
H	2.189745	4.714622	0.000000
H	-1.839154	3.504252	0.000000
O	1.427110	-1.066763	0.000000
C	0.555494	-1.936603	0.000000
N	-0.783677	-1.659894	0.000000
C	-1.737607	-2.641617	0.000000
C	-1.427108	-3.955164	0.000000
C	-0.036032	-4.363905	0.000000
N	0.854828	-3.274222	0.000000
O	0.389850	-5.505034	0.000000
H	-1.049160	-0.667086	0.000000
H	-2.757250	-2.285968	0.000000
H	-2.189744	-4.714626	0.000000
H	1.839155	-3.504256	0.000000

2 U···U pl

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	3.093796	-2.347733	0.052460
C	3.055023	-1.134140	0.047058
N	4.202957	-0.352676	0.060120
C	4.189941	1.013153	0.054337
C	3.033737	1.707657	0.035492
C	1.776657	0.989395	0.020889
N	1.891907	-0.392380	0.027771
O	0.672516	1.532349	0.003387
H	5.068359	-0.866089	0.073990
H	5.157500	1.492676	0.065887
H	3.017303	2.783676	0.031036
H	1.012070	-0.924515	0.018005
O	-0.644165	-1.656982	-0.002472

C	-1.725037	-1.073975	-0.019714
N	-2.910645	-1.775467	-0.033569
C	-4.141205	-1.170807	-0.052948
C	-4.263153	0.170547	-0.059784
C	-3.072128	1.007034	-0.046509
N	-1.869186	0.283051	-0.027008
O	-3.065948	2.224838	-0.051147
H	-2.815475	-2.777039	-0.028381
H	-4.989960	-1.838120	-0.062180
H	-5.227722	0.648071	-0.075607
H	-0.990540	0.819168	-0.016861

3 U···U Calcutta pl

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	3.615875	0.548950	0.000015
C	3.121613	-0.560532	0.000061
N	3.893921	-1.716080	0.000122
C	3.369583	-2.977936	0.000046
C	2.037674	-3.188019	0.000015
C	1.132980	-2.052094	0.000015
N	1.765366	-0.811400	0.000137
O	-0.090164	-2.137802	-0.000076
H	4.888290	-1.562485	0.000015
H	4.087524	-3.784882	0.000000
H	1.623230	-4.181015	-0.000031
H	1.162140	0.020203	0.000076
O	0.099000	1.534225	0.000015
C	-1.128250	1.574326	0.000061
N	-1.774521	2.809372	0.000137
C	-3.133500	3.063904	0.000015
N	-3.890198	1.906906	0.000137
C	-3.351563	0.646591	0.000061
C	-2.019089	0.434479	0.000015
O	-3.615295	4.178787	-0.000137
H	-1.179428	3.626816	0.000061
H	-4.886719	2.047974	0.000015
H	-4.065765	-0.163086	0.000061
H	-1.590225	-0.555893	-0.000031

4 A···A 1 pl

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

N	-1.265244	1.372391	-0.190400
C	-2.112320	0.349915	-0.030212
N	-1.642410	-0.898651	0.146500
C	-2.518463	-1.911591	0.305588
N	-3.847931	-1.874771	0.316788
C	-4.285797	-0.620819	0.138977
C	-3.511475	0.524429	-0.038100
N	-4.287308	1.649368	-0.192795
C	-5.522232	1.183685	-0.109238
N	-5.581223	-0.168518	0.089081
H	-0.251373	1.228226	-0.181686
H	-1.657898	2.287628	-0.318924
H	-2.070007	-2.887680	0.442673
H	-6.413284	1.784058	-0.185745
H	-6.408112	-0.734619	0.182220
N	1.262665	-1.371994	0.185349
C	2.110519	-0.350098	0.025757
N	1.641525	0.898239	-0.154541
C	2.518402	1.910614	-0.313004
N	3.847885	1.873260	-0.320480
C	4.284805	0.619507	-0.139008
C	3.509598	-0.525116	0.038116
N	4.284531	-1.650009	0.197220
C	5.519867	-1.184952	0.116272
N	5.579880	0.166840	-0.084625
H	0.248871	-1.228287	0.174255
H	1.654984	-2.286896	0.317276
H	2.070755	2.886612	-0.453200
H	6.410416	-1.785492	0.196625
H	6.407242	0.732376	-0.176453

5 A···A 2 pl

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.834091	1.181870	-0.413177
C	-1.630188	0.112534	-0.295868
N	-1.103424	-1.092422	-0.018585
C	-1.926819	-2.155426	0.087021
N	-3.249176	-2.207794	-0.046860
C	-3.743240	-0.993408	-0.322464
C	-3.027420	0.194489	-0.461517
N	-3.850800	1.259827	-0.742065
C	-5.055817	0.715591	-0.772110
N	-5.051285	-0.630234	-0.528091
H	0.170395	1.106628	-0.247040

H	-1.268005	2.070511	-0.585861
H	-1.436737	-3.094742	0.311829
H	-5.969147	1.252350	-0.967072
H	-5.846298	-1.246674	-0.500565
N	2.083191	1.031357	0.055344
C	2.975296	0.031906	0.384262
C	2.823837	-1.352234	0.624817
N	3.925140	-2.058182	0.929245
C	5.109833	-1.429794	0.991898
N	5.387833	-0.140549	0.789368
C	4.274124	0.533920	0.489258
N	4.153076	1.875992	0.214355
C	2.836746	2.116776	-0.035934
N	1.646973	-1.989166	0.566742
H	5.952637	-2.061035	1.242340
H	4.906952	2.542740	0.202637
H	2.472565	3.100250	-0.281631
H	1.666641	-2.976242	0.753387
H	0.764526	-1.531845	0.335770

6 A···A 3 pl

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.249039	1.902283	0.402939
C	-2.391342	1.225510	0.591492
N	-3.515381	1.911270	0.849000
C	-4.661346	1.237015	1.042892
N	-4.874191	-0.079697	1.016006
C	-3.736984	-0.731964	0.757202
C	-2.472366	-0.182266	0.537277
N	-1.535141	-1.165253	0.303391
C	-2.229492	-2.290756	0.380554
N	-3.549744	-2.089752	0.648483
H	-1.311081	2.903702	0.446000
H	-0.369446	1.453613	0.160095
H	-5.528122	1.852036	1.246719
H	-1.819275	-3.277939	0.247177
H	-4.263565	-2.791672	0.752838
N	1.291672	-1.903427	-0.199692
C	2.421051	-1.225754	-0.451660
N	3.558060	-1.910950	-0.646194
C	4.690369	-1.236160	-0.906815
N	4.876541	0.080643	-1.011261
C	3.727417	0.732544	-0.810196
C	2.475616	0.182373	-0.527222

N	1.521378	1.165314	-0.376450
C	2.192444	2.291229	-0.568542
N	3.513657	2.090652	-0.831604
H	1.372574	-2.903015	-0.148500
H	0.394791	-1.452423	-0.036072
H	5.569122	-1.850891	-1.052216
H	1.762985	3.278549	-0.528656
H	4.212570	2.792800	-1.008957

7 G···G pl

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.885300	2.220398	0.431564
C	-2.344177	1.122818	0.731216
N	-1.545700	-0.030441	0.604660
C	-1.908798	-1.312424	0.895050
N	-3.095840	-1.653961	1.348236
C	-3.902451	-0.575790	1.487289
C	-3.645752	0.768585	1.225540
N	-4.742340	1.552429	1.502518
C	-5.649887	0.695206	1.925781
N	-5.195694	-0.599823	1.936203
N	-0.967224	-2.266693	0.693451
H	-0.595840	0.152802	0.253616
H	-6.648865	0.949860	2.237366
H	-5.700989	-1.423370	2.216583
H	-1.227676	-3.210754	0.904938
H	-0.039261	-2.071640	0.348450
O	2.010269	-2.197876	-0.341736
C	2.643066	-1.207718	-0.687469
N	3.979828	-1.326370	-1.132965
C	4.793000	-0.300385	-1.545532
N	4.423096	0.953949	-1.579681
C	3.144897	1.123276	-1.160934
C	2.242645	0.161575	-0.725967
N	1.043335	0.725128	-0.385178
C	1.201553	2.017746	-0.606354
N	2.457397	2.303528	-1.076080
N	6.049698	-0.635849	-1.935486
H	4.329605	-2.274963	-1.131271
H	0.434540	2.756378	-0.437149
H	2.818192	3.212097	-1.317566
H	6.652756	0.104858	-2.238861
H	6.386673	-1.576965	-1.930313

8 A···C pl

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.014221	-1.678436	-0.154648
N	-4.382248	-1.352402	-0.226913
C	-4.842239	-0.079910	-0.253891
C	-3.972427	0.957413	-0.210907
C	-2.577545	0.625137	-0.137375
N	-2.141449	-0.625595	-0.111664
O	-2.679214	-2.853043	-0.134354
N	-1.662704	1.602448	-0.091949
H	-5.011566	-2.138504	-0.257919
H	-5.913116	0.050125	-0.310028
H	-4.318665	1.977509	-0.231400
H	-1.959015	2.559631	-0.109543
H	-0.662766	1.366669	-0.039124
N	0.660980	-1.397690	0.037735
C	1.565475	-0.419617	0.082764
N	1.171829	0.871002	0.058426
C	2.105270	1.842300	0.105026
N	3.428864	1.732849	0.175232
C	3.790909	0.441986	0.197922
C	2.952621	-0.670486	0.156738
N	3.662155	-1.848114	0.197510
C	4.920242	-1.446747	0.262817
N	5.056641	-0.085480	0.266190
H	-0.339920	-1.185455	-0.015671
H	0.983017	-2.348816	0.057449
H	1.715927	2.853027	0.081635
H	5.773697	-2.102264	0.309738
H	5.913116	0.441025	0.310013

9 A···T WC

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.758575	0.389297	0.087600
C	-1.430756	-0.773193	0.072281
C	-2.837738	-0.711838	0.058441
C	-3.403122	0.563065	0.065048
N	-2.759094	1.737457	0.082413
C	-1.441910	1.553589	0.092148
N	-3.795547	-1.698669	0.037811
C	-4.931595	-1.021698	0.032379
N	-4.757065	0.334717	0.048325

N	-0.759354	-1.933243	0.079422
H	-0.823135	2.441910	0.105209
H	-5.912643	-1.466110	0.017044
H	-5.473679	1.041306	0.047546
H	0.255341	-1.937775	0.037216
H	-1.283447	-2.786835	0.020889
N	4.022537	1.809372	0.057907
C	4.782715	0.669922	0.006241
C	4.231842	-0.563858	-0.024628
C	2.779449	-0.659698	-0.001083
N	2.097794	0.542145	0.052094
C	2.638794	1.807831	0.082657
C	5.025635	-1.826218	-0.081070
O	2.172379	-1.732132	-0.026306
O	1.980118	2.831482	0.127029
H	4.450684	2.719742	0.079453
H	5.852844	0.822098	-0.008392
H	1.057022	0.495422	0.069611
H	4.800919	-2.457642	0.777069
H	4.769104	-2.399445	-0.970627
H	6.092712	-1.614075	-0.093430

10 A···T WC (C_1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.735062	-0.072144	-0.434952
C	1.474014	-0.079941	0.686356
C	2.874847	-0.053619	0.543365
C	3.364670	-0.024643	-0.762054
N	2.653183	-0.018372	-1.897034
C	1.349106	-0.042923	-1.636871
N	3.888641	-0.049606	1.472870
C	4.983047	-0.018784	0.731110
N	4.729523	-0.002945	-0.612778
N	0.871674	-0.120697	1.883057
H	0.679474	-0.039154	-2.487640
H	5.988312	-0.006622	1.117798
H	5.403580	0.020691	-1.359741
H	-0.141251	-0.086548	1.947830
H	1.444443	-0.078903	2.705811
N	-4.121078	-0.045135	-1.572418
C	-4.813600	-0.027283	-0.389709
C	-4.191635	-0.022247	0.810226
C	-2.736053	-0.036713	0.820587
N	-2.125565	-0.055222	-0.419952

C	-2.739502	-0.059113	-1.652298
C	-4.910522	-0.002853	2.117783
O	-2.067383	-0.032974	1.855988
O	-2.141586	-0.073349	-2.713440
H	-4.601639	-0.047775	-2.456543
H	-5.890839	-0.017242	-0.478775
H	-1.083740	-0.065781	-0.434479
H	-4.643845	-0.874405	2.713455
H	-4.626633	0.874405	2.696945
H	-5.988312	0.006363	1.968643

11 mA···mT H

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.396988	-2.744461	-0.051865
C	2.390045	-1.842697	-0.041000
N	3.663055	-2.265930	-0.032898
C	4.655716	-1.359329	-0.024155
N	4.574509	-0.027176	-0.021606
C	3.296021	0.364349	-0.029816
C	2.163100	-0.450607	-0.039856
N	1.021011	0.310104	-0.045502
C	1.458694	1.563553	-0.039261
N	2.816254	1.653549	-0.029465
C	3.627960	2.852798	-0.022614
H	1.655457	-3.714584	-0.042908
H	0.416641	-2.483353	-0.046021
H	5.655900	-1.772964	-0.017960
H	0.814285	2.428925	-0.040833
H	4.265000	2.861053	0.857620
H	4.253433	2.880890	-0.910812
H	2.969421	3.715973	-0.008682
N	-1.744125	-0.080017	-0.050110
C	-2.441360	1.101700	-0.044388
N	-3.817902	0.955963	-0.041107
C	-4.405212	-0.282867	-0.027100
C	-3.706497	-1.443420	-0.025070
C	-2.258102	-1.359940	-0.036240
O	-1.904526	2.202377	-0.042862
O	-1.511627	-2.342606	-0.035370
C	-4.348175	-2.791290	-0.013489
C	-4.605316	2.179138	-0.024170
H	-0.704391	0.017746	-0.052658
H	-5.487045	-0.275970	-0.019547
H	-4.047256	-3.365082	-0.888626

H	-5.432877	-2.704727	-0.003983
H	-4.031204	-3.357239	0.861053
H	-4.297958	2.825150	-0.841248
H	-4.457306	2.714172	0.910812
H	-5.651840	1.913589	-0.134796

12 G···A 1

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	-1.279831	2.501328	-0.269700
C	-2.105331	1.592972	-0.367508
N	-1.695267	0.253479	-0.318237
C	-2.499100	-0.836563	-0.459839
N	-3.795715	-0.792038	-0.632538
C	-4.244690	0.487213	-0.643784
C	-3.526230	1.676224	-0.536285
N	-4.352341	2.771484	-0.617722
C	-5.554367	2.250107	-0.770798
N	-5.544998	0.878708	-0.794708
N	-1.861877	-2.055679	-0.356339
H	-0.688538	0.088364	-0.120438
H	-6.467056	2.812851	-0.869278
H	-6.332962	0.261841	-0.901321
H	-2.439651	-2.812851	-0.685272
H	-0.923416	-2.075928	-0.724472
N	1.462723	1.905151	-0.659485
C	1.936432	0.732376	-0.225555
N	1.087265	-0.245331	0.148941
C	1.584869	-1.419678	0.593582
N	2.853958	-1.794708	0.711456
C	3.675827	-0.811691	0.316803
C	3.315979	0.451218	-0.152435
N	4.415771	1.217957	-0.454315
C	5.432205	0.420990	-0.171356
N	5.047577	-0.806595	0.293930
H	0.476898	2.149155	-0.526657
H	2.134094	2.629745	-0.844940
H	0.840637	-2.144608	0.900757
H	6.470612	0.683411	-0.285217
H	5.645600	-1.565628	0.576050

13 G···A 1 pl

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
N	-1.457260	-0.212509	0.000000
C	-2.071213	-1.414490	0.000000
N	-3.367691	-1.699493	0.000000
C	-4.097778	-0.575424	0.000000
C	-3.619339	0.732346	0.000000
C	-2.218491	0.902817	0.000000
N	-5.463257	-0.442566	0.000000
C	-5.730194	0.899400	0.000000
N	-4.642319	1.649643	0.000000
N	-1.658295	2.112671	0.000000
H	-1.415421	-2.277557	0.000000
H	-6.130661	-1.196106	0.000000
H	-6.739136	1.275940	0.000000
H	-2.271515	2.908447	0.000000
H	-0.642593	2.243408	0.000000
C	2.278519	-0.888367	0.000000
N	1.481888	0.220581	0.000000
C	1.926453	1.551819	0.000000
C	3.355728	1.607712	0.000000
C	4.058945	0.405640	0.000000
N	3.588943	-0.863327	0.000000
N	5.374619	0.773239	0.000000
C	5.407318	2.145523	0.000000
N	4.206192	2.687805	0.000000
N	1.632645	-2.082382	0.000000
O	1.115662	2.477997	0.000000
H	0.458481	0.084549	0.000000
H	6.157852	0.141510	0.000000
H	6.335754	2.690704	0.000000
H	0.633911	-2.134186	0.000000
H	2.185440	-2.917206	0.000000

14 G···A 2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	5.503265	-1.484985	-0.137146
C	4.370590	-1.069611	0.030289
N	3.299042	-1.623718	-0.755295
C	1.972290	-1.274521	-0.714127
N	1.512405	-0.338654	0.101028
C	2.478577	0.207809	0.883881
C	3.844818	-0.069183	0.921722
N	4.482574	0.709442	1.869781
C	3.531158	1.435471	2.393341

N	2.289000	1.178970	1.832520
N	1.122040	-1.895828	-1.569092
H	3.615707	-2.327942	-1.410416
H	3.655304	2.168991	3.178009
H	1.402176	1.582993	2.093567
H	0.115891	-1.814667	-1.375153
H	1.428421	-2.740692	-2.025085
N	-1.045670	1.202408	-0.317932
C	-2.297409	0.732635	-0.474686
N	-3.327377	1.593964	-0.330368
C	-4.579437	1.139679	-0.475830
N	-4.995850	-0.101349	-0.751923
C	-3.956711	-0.929337	-0.902649
C	-2.597519	-0.615189	-0.795715
N	-1.815582	-1.736450	-1.044128
C	-2.679749	-2.695831	-1.283859
N	-3.984146	-2.274185	-1.210693
H	-0.961380	2.184174	-0.104355
H	-0.223923	0.597183	-0.260773
H	-5.362076	1.884400	-0.346848
H	-2.424911	-3.720016	-1.519180
H	-4.815811	-2.825684	-1.359634

15 G···A 2 pl

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.803009	-1.277725	0.000000
N	1.514786	0.005783	0.000000
C	2.631149	0.782181	0.000000
C	3.971497	0.410187	0.000000
C	4.294067	-0.989304	0.000000
N	3.088638	-1.747314	0.000000
N	0.814850	-2.194717	0.000000
N	4.798859	1.506912	0.000000
C	3.971863	2.531600	0.000000
N	2.652725	2.149460	0.000000
O	5.366562	-1.562729	0.000000
H	3.249039	-2.744965	0.000000
H	-0.161713	-1.896851	0.000000
H	1.030548	-3.172409	0.000000
H	4.262711	3.567703	0.000000
H	1.850403	2.755646	0.000000
C	-2.975586	-2.461349	0.000000
N	-2.050873	-1.513107	0.000000
C	-2.774353	-0.339676	0.000000

N	-4.244370	-1.969040	0.000000
C	-4.146942	-0.597534	0.000000
C	-2.400436	1.020706	0.000000
N	-3.376282	1.939056	0.000000
C	-4.657806	1.536423	0.000000
N	-5.140839	0.293564	0.000000
N	-1.124359	1.438461	0.000000
H	-2.773697	-3.518997	0.000000
H	-5.101639	-2.497040	0.000000
H	-5.391739	2.331741	0.000000
H	-0.322571	0.811935	0.000000
H	-0.990295	2.433914	0.000000

16 G···A 3

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	0.893784	-1.944611	-0.547882
C	1.636475	-0.987717	-0.338470
N	1.098434	0.281296	-0.079941
C	1.802948	1.410156	0.204346
N	3.107620	1.486191	0.249634
C	3.677582	0.287720	-0.034592
C	3.069733	-0.934998	-0.312714
N	4.001434	-1.921951	-0.524628
C	5.157272	-1.303177	-0.377151
N	5.018173	0.028351	-0.080017
N	1.037460	2.545975	0.405975
H	0.070419	0.368820	-0.169815
H	6.125244	-1.764847	-0.473221
H	5.750061	0.700592	0.078690
H	1.581116	3.282181	0.829636
H	0.169418	2.371933	0.890640
N	-1.796921	-2.302200	0.342682
C	-2.867218	-1.516464	0.143387
N	-4.095200	-2.043533	0.269989
C	-5.169600	-1.262680	0.072540
N	-5.219100	0.029556	-0.258667
C	-3.985626	0.529465	-0.364517
C	-2.776932	-0.141449	-0.170334
N	-1.709244	0.713196	-0.346313
C	-2.266006	1.876694	-0.656036
N	-3.624252	1.819748	-0.680130
H	-1.997406	-3.282166	0.451477
H	-0.869293	-2.046509	0.005798
H	-6.125244	-1.756073	0.192413

H	-1.717072	2.777710	-0.875458
H	-4.259735	2.571732	-0.890640

17 G···A 4

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	5.974731	-1.842682	0.217239
C	4.921860	-1.236877	0.165176
N	3.691528	-1.939758	0.318802
C	2.424454	-1.426392	0.302292
N	2.179352	-0.145859	0.127411
C	3.318054	0.577881	-0.039825
C	4.644196	0.158707	-0.038391
N	5.504303	1.209335	-0.247955
C	4.708084	2.251907	-0.376663
N	3.379837	1.926086	-0.257111
N	1.400040	-2.289749	0.528961
H	3.816681	-2.927612	0.492020
H	5.030045	3.263412	-0.556244
H	2.592361	2.546524	-0.343475
H	0.467468	-1.961014	0.253082
H	1.580811	-3.263397	0.355728
N	-0.604004	0.784058	0.544464
C	-1.583832	-0.059845	0.192352
N	-1.285797	-1.313568	-0.190628
C	-2.288269	-2.143982	-0.546387
N	-3.596710	-1.909012	-0.575409
C	-3.861710	-0.656448	-0.181000
C	-2.941452	0.314636	0.211243
N	-3.555725	1.497467	0.549057
C	-4.839447	1.239090	0.362900
N	-5.080627	-0.034363	-0.074326
H	0.374084	0.507996	0.452240
H	-0.865021	1.704681	0.847992
H	-1.976868	-3.136017	-0.847992
H	-5.639084	1.941162	0.529846
H	-5.974731	-0.447388	-0.282074

18 G···C WC

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.366226	1.403473	-0.643295
N	3.725449	1.549881	-0.941879

C	4.544907	0.497528	-1.181458
C	4.058060	-0.764465	-1.133347
C	2.663528	-0.910049	-0.824341
N	1.872513	0.136658	-0.601181
O	1.693649	2.412735	-0.435867
N	2.119232	-2.125320	-0.755402
H	4.065430	2.497803	-0.970093
H	5.577087	0.724747	-1.403091
H	4.693359	-1.614853	-1.318390
H	2.692780	-2.934906	-0.899536
H	1.129333	-2.235962	-0.495041
O	-0.555038	-2.406158	-0.009949
C	-1.369217	-1.494415	0.161591
N	-0.988098	-0.160690	-0.018875
C	-1.787140	0.940704	0.132828
N	-3.051453	0.883286	0.494003
C	-3.457489	-0.391846	0.680008
C	-2.743454	-1.580933	0.545517
N	-3.527603	-2.676697	0.826065
C	-4.700623	-2.155197	1.126328
N	-4.712708	-0.784470	1.054642
N	-1.216705	2.135100	-0.157761
H	0.002686	-0.017731	-0.263809
H	-5.577087	-2.716156	1.403091
H	-5.486603	-0.167221	1.234055
H	-1.748428	2.934906	0.134415
H	-0.204987	2.225037	-0.203140

19 mG···mC WC

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.044083	0.733856	-0.005081
N	-4.419983	0.457504	-0.009750
C	-4.872314	-0.815384	0.082764
C	-4.016922	-1.863434	0.181366
C	-2.619629	-1.561386	0.183792
N	-2.179962	-0.307190	0.099731
O	-2.686920	1.912643	-0.096893
N	-1.712769	-2.535126	0.275803
C	-5.324982	1.591675	-0.118073
H	-5.945800	-0.940948	0.071198
H	-4.385590	-2.873810	0.251678
H	-2.016220	-3.490112	0.312637
H	-0.705826	-2.317276	0.222595
H	-5.130753	2.132568	-1.039886

H	-5.168076	2.270600	0.715240
H	-6.345000	1.219467	-0.110397
O	0.979019	-1.946091	0.094559
C	1.476120	-0.814377	0.130463
N	0.656174	0.315094	0.207458
C	1.071198	1.618729	0.260498
N	2.334808	1.984329	0.227478
C	3.160706	0.917100	0.150696
C	2.854858	-0.443069	0.103500
N	3.992935	-1.208191	0.031342
C	4.967560	-0.317078	0.034821
N	4.524796	0.980148	0.105133
N	0.094131	2.548233	0.400696
C	5.313232	2.192078	0.130142
H	-0.358841	0.124344	0.203200
H	6.020400	-0.543869	-0.011368
H	0.394684	3.494400	0.249802
H	-0.870773	2.315292	0.173630
H	5.072678	2.813583	-0.728700
H	5.106949	2.752502	1.038376
H	6.364487	1.920547	0.100067

20 G···U wobble

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.735900	-1.836502	0.145096
C	-1.533615	-0.901840	0.243759
N	-1.070007	0.418488	0.219727
C	-1.829086	1.547409	0.317505
N	-3.133545	1.552551	0.451584
C	-3.626648	0.290756	0.479950
C	-2.957000	-0.929413	0.389465
N	-3.829544	-1.989624	0.460297
C	-5.010300	-1.418625	0.591751
N	-4.943939	-0.047562	0.609222
N	-1.142609	2.717484	0.267776
H	-0.052933	0.526260	0.116745
H	-5.947128	-1.942154	0.678650
H	-5.707092	0.602158	0.699097
H	-1.680908	3.575165	0.136185
H	-0.145600	2.728897	0.164413
O	1.658951	0.813141	-0.056030
C	2.418457	-0.157043	-0.152679
N	2.017639	-1.456436	-0.133850
C	2.845139	-2.592682	-0.240677

C	4.261047	-2.283188	-0.383209
C	4.670273	-1.001419	-0.403030
N	3.773453	0.032257	-0.290985
O	2.370834	-3.711884	-0.210983
H	0.997604	-1.631973	-0.030746
H	4.958252	-3.098663	-0.470551
H	5.705597	-0.713684	-0.506332
H	4.074936	0.991882	-0.305374

21 water···MeOH

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.525330	-0.050971	-0.314517
H	-0.942007	0.747902	0.011253
H	0.403697	0.059786	-0.073568
O	2.316633	0.045501	0.071858
C	2.781638	-0.426129	-1.190301
H	2.684616	-0.526577	0.749387
H	2.350821	0.224965	-1.943415
H	3.867602	-0.375336	-1.264613
H	2.453296	-1.445999	-1.389381

22 water···$MeNH_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.687465	-0.111744	-0.019625
H	-1.046122	0.775938	0.012707
H	0.274043	0.025851	-0.003497
N	2.233976	0.103183	0.005854
C	2.893311	1.411547	-0.034388
H	2.529341	-0.449455	-0.788937
H	2.544057	-0.407538	0.822713
H	2.582769	1.993272	0.830127
H	3.984621	1.372252	-0.043344
H	2.566599	1.947464	-0.922212

23 water···Peptide

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.392018	-0.384719	0.076071
H	-0.911461	0.413812	0.177649
H	0.524904	-0.068485	0.090511

C	2.197705	-2.245403	-0.230313
C	2.952437	-0.947391	-0.097720
O	2.375722	0.127904	0.058869
N	4.303070	-1.044893	-0.162338
C	5.171313	0.107077	-0.052895
H	2.847668	-3.106515	-0.363229
H	1.516729	-2.167931	-1.074179
H	1.584688	-2.384199	0.656695
H	4.704022	-1.955427	-0.291853
H	4.534818	0.975378	0.081890
H	5.836902	0.015622	0.803198
H	5.765778	0.236498	-0.955154

24 MeOH···MeOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	-0.636135	-0.023282	0.280599
C	-1.152065	-1.311288	0.015260
H	0.308097	-0.047079	0.076464
H	-2.209945	-1.296265	0.263956
H	-1.056610	-1.592671	-1.036191
H	-0.674836	-2.086273	0.620511
O	2.210419	-0.122122	-0.012103
C	2.719253	0.034897	1.309615
H	2.679209	0.492263	-0.581769
H	2.165684	-0.653299	1.939746
H	3.778249	-0.215542	1.366338
H	2.566814	1.045591	1.687507

25 MeOH···peptide

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	-0.208777	-0.216871	-1.032406
C	-1.022173	-0.741171	-0.005454
H	0.711126	-0.386892	-0.773962
H	-2.057491	-0.538707	-0.268597
H	-0.907743	-1.821826	0.108537
H	-0.824631	-0.275495	0.964645
C	1.973490	1.903224	0.432301
C	2.889121	0.748285	0.116385
O	2.464926	-0.371626	-0.168697
N	4.215258	1.010009	0.175584
C	5.197664	-0.030102	-0.047159

H	2.479884	2.864673	0.397431
H	1.562946	1.757088	1.430178
H	1.143843	1.893711	-0.269204
H	4.513270	1.920438	0.473272
H	4.841107	-0.681039	-0.839336
H	6.138033	0.423422	-0.345673
H	5.357174	-0.634629	0.844916

26 MeOH···water

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	-0.786562	0.045168	-0.007189
C	-1.247991	-1.290284	0.001084
H	0.177707	0.012696	-0.006835
H	-2.334277	-1.258897	0.000221
H	-0.925966	-1.849768	-0.880445
H	-0.927028	-1.838463	0.890077
O	2.128883	-0.051337	-0.004741
H	2.568087	0.336816	-0.764614
H	2.566767	0.351268	0.748349

27 $MeNH_2$···peptide

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.569708	0.814372	0.101098
C	-0.305514	0.065710	1.328792
H	0.130878	0.561411	-0.587615
H	-1.461252	0.526915	-0.280430
H	-1.057149	0.314270	2.075959
H	-0.288024	-1.022292	1.214846
H	0.660458	0.368509	1.730242
C	2.256892	2.690100	-0.149327
C	2.768883	1.272302	-0.147033
O	2.308903	0.406566	-0.886208
N	3.755366	0.999270	0.745297
C	4.343812	-0.320321	0.822797
H	2.381510	3.101277	-1.148372
H	2.763463	3.331092	0.568457
H	1.190480	2.663570	0.069094
H	4.155127	1.754203	1.270650
H	3.555635	-1.061651	0.729776
H	5.065071	-0.492316	0.024253
H	4.838465	-0.436189	1.782737

28 $MeNH_2$···water

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.533464	-0.279594	0.106996
C	-1.016909	0.588486	1.187373
H	-0.629151	-1.248425	0.382849
H	-1.122604	-0.166159	-0.707764
H	-0.912760	1.625552	0.879521
H	-2.054737	0.415082	1.478504
H	-0.385023	0.448801	2.060614
O	2.093268	0.917311	0.212097
H	1.275751	0.421039	0.038944
H	2.675170	0.658813	-0.503649

29 peptide···MeOH

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-0.849317	-0.339499	2.491717
C	-1.564032	-0.353323	1.159475
O	-2.749526	-0.651538	1.056761
N	-0.801654	-0.027355	0.088342
C	-1.385350	-0.002351	-1.234137
H	0.184344	-0.011047	2.416185
H	-0.882498	-1.342051	2.912703
H	-1.390803	0.316878	3.168429
H	0.161188	0.240360	0.218714
H	-1.891617	-0.942801	-1.440096
H	-2.119972	0.796212	-1.330880
H	-0.594646	0.149571	-1.963128
O	2.137066	0.252017	0.453719
C	2.656150	-1.053348	0.687601
H	2.857921	0.879317	0.544134
H	1.823578	-1.742136	0.582024
H	3.422289	-1.322341	-0.039280
H	3.064247	-1.154797	1.693235

30 peptide···$MeNH_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-0.778573	-0.463321	2.490388
C	-1.520503	-0.456628	1.172325

O	-2.700835	-0.783586	1.089597
N	-0.791954	-0.069640	0.100589
C	-1.397798	-0.056082	-1.211318
H	0.224745	-0.050953	2.413484
H	-0.722480	-1.487092	2.854585
H	-1.351908	0.110817	3.213684
H	0.194112	0.145708	0.202925
H	-2.314928	0.528891	-1.199710
H	-0.698804	0.387261	-1.915366
H	-1.652982	-1.061529	-1.545435
N	2.238288	0.254574	0.282519
C	2.610591	-1.156609	0.436272
H	2.641955	0.794494	1.037719
H	2.656292	0.621956	-0.563127
H	2.184304	-1.727641	-0.385103
H	3.685990	-1.343298	0.462055
H	2.176118	-1.541016	1.356108

31 peptide···peptide

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.701503	-0.290628	2.406884
C	-1.448546	-0.244877	1.091815
O	-2.660450	-0.428479	1.034346
N	-0.670057	0.005917	0.009777
C	-1.227055	0.089794	-1.319968
H	-1.183296	0.395648	3.098874
H	0.349562	-0.030322	2.307833
H	-0.794057	-1.291605	2.824039
H	0.326675	0.122564	0.141593
H	-2.292024	-0.106501	-1.240878
H	-1.077802	1.079940	-1.748544
H	-0.776628	-0.647999	-1.983373
C	2.041775	-2.351698	0.686398
C	2.809411	-1.097286	0.350161
O	2.264224	0.004151	0.293188
N	4.136169	-1.266100	0.136413
C	5.023407	-0.159634	-0.152536
H	2.600000	-3.261701	0.480490
H	1.113083	-2.358227	0.122072
H	1.782556	-2.328251	1.743339
H	4.512490	-2.193345	0.213170
H	4.409215	0.731176	-0.232359
H	5.750822	-0.020168	0.644868
H	5.548398	-0.319615	-1.091678

32 peptide···water

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-0.724305	-0.704936	2.283868
C	-1.614935	-0.387429	1.104069
O	-2.837324	-0.415022	1.194133
N	-0.953420	-0.076404	-0.040820
C	-1.658124	0.250094	-1.258553
H	0.335318	-0.629943	2.053182
H	-0.951697	-1.711990	2.625651
H	-0.969628	-0.022080	3.093765
H	0.053809	-0.075567	-0.036640
H	-2.720372	0.176944	-1.046653
H	-1.430305	1.262963	-1.588094
H	-1.405626	-0.444335	-2.058584
O	2.102777	-0.058407	-0.155077
H	2.667754	-0.771366	-0.460276
H	2.682529	0.705787	-0.131178

33 MeOH···pyridine

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.627652	0.087467	0.001471
C	-0.977931	-1.278556	0.001238
H	0.343602	0.122303	-0.000600
H	-2.063392	-1.342043	0.005009
H	-0.614884	-1.806376	-0.885384
H	-0.608640	-1.808237	0.884173
N	2.272337	0.016432	-0.001627
C	2.968705	-0.008003	-1.146346
C	4.358342	-0.057746	-1.195032
C	5.068715	-0.083459	0.000581
C	4.356468	-0.058437	1.195121
C	2.966914	-0.008688	1.144167
H	2.384226	0.015221	-2.057322
H	4.865694	-0.075038	-2.148814
H	6.149051	-0.121223	0.001431
H	4.862267	-0.076262	2.149607
H	2.380908	0.013987	2.054286

34 AcOH···U

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.113626	1.327020	0.275167
O	-0.467083	2.349388	0.461537
O	-0.578089	0.136920	0.049617
C	-2.611425	1.286190	0.277361
H	0.413320	0.203257	0.055487
H	-3.006649	2.276885	0.465790
H	-2.964256	0.915259	-0.682001
H	-2.953114	0.591798	1.041240
N	4.188697	1.087953	0.182882
C	5.110225	2.136069	0.364335
O	6.307372	1.917773	0.311455
C	4.471159	3.415531	0.604942
C	3.124075	3.495522	0.634323
N	2.320344	2.404840	0.443917
C	2.820277	1.154617	0.209745
O	2.108244	0.165112	0.036275
H	4.581902	0.172563	0.011162
H	5.090694	4.282456	0.756419
H	2.601235	4.423969	0.809621
H	1.296292	2.474787	0.467707

35 $AcNH_2\cdots U$

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.232727	1.211639	-0.141624
O	-0.571277	2.242016	0.025617
N	-0.670581	0.003889	-0.314281
C	-2.738245	1.266758	-0.155887
H	0.343847	-0.090560	-0.308327
H	-1.244214	-0.806324	-0.446683
H	-3.077975	1.646605	0.804502
H	-3.202115	0.302865	-0.346211
H	-3.049987	1.975490	-0.918597
N	4.195213	1.117429	-0.119542
C	4.998839	2.260274	0.030940
O	6.214401	2.164651	0.015755
C	4.226247	3.475590	0.194084
C	2.877086	3.413915	0.188407
N	2.192004	2.241633	0.033841
C	2.822894	1.037164	-0.128419
O	2.225705	-0.026752	-0.270226
H	4.685242	0.241471	-0.237480
H	4.748010	4.408783	0.317119

H	2.256682	4.290275	0.306084
H	1.159213	2.232572	0.033004

36 A A st

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.900000	-0.357920	0.000000
C	-1.900000	0.980880	0.000000
N	-0.849764	1.832930	0.000000
C	0.388696	1.313959	0.000000
C	0.540366	-0.087960	0.000000
C	-0.642749	-0.832327	0.000000
N	-0.218407	-2.143469	0.000000
C	1.153286	-2.119668	0.000000
N	1.661233	-0.894706	0.000000
N	1.454508	2.146930	0.000000
H	-2.878574	1.456419	0.000000
H	-0.820187	-2.958723	0.000000
H	1.738777	-3.030641	0.000000
H	1.299076	3.144190	0.000000
H	2.391812	1.773376	0.000000
N	2.040033	1.024408	3.300000
C	3.199467	0.355008	3.300000
N	3.412246	-0.980548	3.300000
C	2.343574	-1.793600	3.300000
C	1.053641	-1.223991	3.300000
C	1.000558	0.172801	3.300000
N	-0.347095	0.460881	3.300000
C	-1.012329	-0.738940	3.300000
N	-0.205455	-1.791317	3.300000
N	2.532041	-3.133106	3.300000
H	4.100583	0.964708	3.300000
H	-0.752235	1.389665	3.300000
H	-2.094000	-0.790504	3.300000
H	3.473410	-3.497128	3.300000
H	1.739882	-3.758058	3.300000

37 G G st

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	0.239288	-2.692059	0.000000
C	0.239288	-1.466459	0.000000
N	1.483165	-0.758572	0.000000
C	1.658539	0.604997	0.000000

N	0.669409	1.469841	0.000000
C	-0.542407	0.843961	0.000000
C	-0.843309	-0.517176	0.000000
N	-2.204411	-0.736751	0.000000
C	-2.720320	0.481621	0.000000
N	-1.762104	1.468724	0.000000
N	2.942972	1.061961	0.000000
H	2.289438	-1.378256	0.000000
H	-3.778048	0.711408	0.000000
H	-1.905514	2.471825	0.000000
H	3.081601	2.060888	0.000000
H	3.744241	0.452524	0.000000
O	-3.492712	1.031819	3.300000
C	-2.285732	0.818995	3.300000
N	-1.804596	-0.528908	3.300000
C	-0.492196	-0.938399	3.300000
N	0.531269	-0.114475	3.300000
C	0.125328	1.187614	3.300000
C	-1.162879	1.720304	3.300000
N	-1.142766	3.098856	3.300000
C	0.146684	3.395359	3.300000
N	0.952397	2.280292	3.300000
N	-0.265214	-2.282670	3.300000
H	-2.554874	-1.215325	3.300000
H	0.556652	4.397116	3.300000
H	1.965161	2.247337	3.300000
H	0.694464	-2.592654	3.300000
H	-1.004532	-2.965938	3.300000

38 C C st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.221000	-0.448800	0.000000
N	-1.221000	0.968600	0.000000
C	-0.096454	1.723449	0.000000
C	1.127070	1.116940	0.000000
C	1.112692	-0.322388	0.000000
N	0.014110	-1.055259	0.000000
O	-2.294878	-1.037591	0.000000
N	2.297645	-0.991871	0.000000
H	-2.144657	1.393736	0.000000
H	-0.229047	2.806160	0.000000
H	2.047734	1.697075	0.000000
H	3.183948	-0.509430	0.000000
H	2.274439	-2.004205	0.000000

C	0.821000	1.448800	3.300000
N	0.821000	0.031400	3.300000
C	-0.303546	-0.723449	3.300000
C	-1.527070	-0.116940	3.300000
C	-1.512692	1.322388	3.300000
N	-0.414110	2.055259	3.300000
O	1.894878	2.037592	3.300000
N	-2.697645	1.991870	3.300000
H	1.744657	-0.393735	3.300000
H	-0.170952	-1.806160	3.300000
H	-2.447734	-0.697076	3.300000
H	-3.583949	1.509429	3.300000
H	-2.674440	3.004204	3.300000

39 A C st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-1.900000	-0.357920	0.000000
C	-1.900000	0.980880	0.000000
N	-0.849764	1.832930	0.000000
C	0.388696	1.313959	0.000000
C	0.540366	-0.087960	0.000000
C	-0.642749	-0.832327	0.000000
N	-0.218407	-2.143469	0.000000
C	1.153286	-2.119668	0.000000
N	1.661233	-0.894706	0.000000
N	1.454508	2.146930	0.000000
H	-2.878574	1.456419	0.000000
H	-0.820187	-2.958723	0.000000
H	1.738777	-3.030641	0.000000
H	1.299076	3.144190	0.000000
H	2.391812	1.773376	0.000000
C	0.248177	-2.184700	3.300000
N	0.937510	-0.946216	3.300000
C	0.322022	0.260256	3.300000
C	-1.042025	0.325350	3.300000
C	-1.729460	-0.939287	3.300000
N	-1.125970	-2.113930	3.300000
O	0.900151	-3.221435	3.300000
N	-3.090432	-0.947978	3.300000
H	1.951333	-1.023952	3.300000
H	0.964440	1.141814	3.300000
H	-1.564335	1.280007	3.300000
H	-3.630229	-0.095393	3.300000
H	-3.562489	-1.843814	3.300000

40 A U st

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.900000	-0.357920	0.000000
C	-1.900000	0.980880	0.000000
N	-0.849764	1.832930	0.000000
C	0.388696	1.313959	0.000000
C	0.540366	-0.087960	0.000000
C	-0.642749	-0.832327	0.000000
N	-0.218407	-2.143469	0.000000
C	1.153286	-2.119668	0.000000
N	1.661233	-0.894706	0.000000
N	1.454508	2.146930	0.000000
H	-2.878574	1.456419	0.000000
H	-0.820187	-2.958723	0.000000
H	1.738777	-3.030641	0.000000
H	1.299076	3.144190	0.000000
H	2.391812	1.773376	0.000000
O	0.829054	-2.734942	3.300000
C	0.618008	-1.525700	3.300000
N	1.688238	-0.611702	3.300000
C	1.647378	0.773190	3.300000
N	0.348300	1.265366	3.300000
C	-0.774655	0.468238	3.300000
C	-0.688580	-0.880715	3.300000
O	2.637068	1.493245	3.300000
H	2.620301	-1.018658	3.300000
H	0.274546	2.275733	3.300000
H	-1.721660	0.998110	3.300000
H	-1.570866	-1.507328	3.300000

41 G A st

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	0.239288	-2.692058	0.000000
C	0.239288	-1.466458	0.000000
N	1.483165	-0.758571	0.000000
C	1.658539	0.604998	0.000000
N	0.669409	1.469842	0.000000
C	-0.542407	0.843962	0.000000
C	-0.843309	-0.517175	0.000000
N	-2.204411	-0.736750	0.000000
C	-2.720320	0.481622	0.000000

N	-1.762104	1.468725	0.000000
N	2.942972	1.061962	0.000000
H	2.289438	-1.378255	0.000000
H	-3.778048	0.711409	0.000000
H	-1.905514	2.471825	0.000000
H	3.081601	2.060889	0.000000
H	3.744241	0.452525	0.000000
N	-2.933441	0.997694	-3.300000
C	-2.687167	2.313648	-3.300000
N	-1.498117	2.957965	-3.300000
C	-0.376257	2.220036	-3.300000
C	-0.485059	0.814139	-3.300000
C	-1.784912	0.300109	-3.300000
N	-1.608998	-1.066717	-3.300000
C	-0.256333	-1.295646	-3.300000
N	0.468279	-0.185024	-3.300000
N	0.824594	2.842734	-3.300000
H	-3.561566	2.961082	-3.300000
H	-2.350475	-1.757360	-3.300000
H	0.151592	-2.298775	-3.300000
H	0.855261	3.851568	-3.300000
H	1.677188	2.303137	-3.300000

42 G C st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	0.239288	-2.692058	0.000000
C	0.239288	-1.466458	0.000000
N	1.483165	-0.758571	0.000000
C	1.658539	0.604998	0.000000
N	0.669409	1.469842	0.000000
C	-0.542407	0.843962	0.000000
C	-0.843309	-0.517175	0.000000
N	-2.204411	-0.736750	0.000000
C	-2.720320	0.481622	0.000000
N	-1.762104	1.468725	0.000000
N	2.942972	1.061962	0.000000
H	2.289438	-1.378255	0.000000
H	-3.778048	0.711409	0.000000
H	-1.905514	2.471825	0.000000
H	3.081601	2.060889	0.000000
H	3.744241	0.452525	0.000000
C	2.514074	0.521273	-3.300000
N	1.226353	1.113594	-3.300000
C	0.070641	0.407387	-3.300000

C	0.110357	-0.957636	-3.300000
C	1.423994	-1.546050	-3.300000
N	2.548890	-0.854247	-3.300000
O	3.497750	1.250843	-3.300000
N	1.537042	-2.902348	-3.300000
H	1.226102	2.130394	-3.300000
H	-0.857593	0.980299	-3.300000
H	-0.801428	-1.551627	-3.300000
H	0.728369	-3.505947	-3.300000
H	2.466444	-3.304307	-3.300000

43 G U st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
O	0.239288	-2.692058	0.000000
C	0.239288	-1.466458	0.000000
N	1.483165	-0.758571	0.000000
C	1.658539	0.604998	0.000000
N	0.669409	1.469842	0.000000
C	-0.542407	0.843962	0.000000
C	-0.843309	-0.517175	0.000000
N	-2.204411	-0.736750	0.000000
C	-2.720320	0.481622	0.000000
N	-1.762104	1.468725	0.000000
N	2.942972	1.061962	0.000000
H	2.289438	-1.378255	0.000000
H	-3.778048	0.711409	0.000000
H	-1.905514	2.471825	0.000000
H	3.081601	2.060889	0.000000
H	3.744241	0.452525	0.000000
O	2.727493	0.028428	-3.300000
C	1.538020	-0.274928	-3.300000
N	0.544481	0.721899	-3.300000
C	-0.833176	0.574733	-3.300000
N	-1.224065	-0.758325	-3.300000
C	-0.342999	-1.816702	-3.300000
C	0.995351	-1.627218	-3.300000
O	-1.627156	1.506162	-3.300000
H	0.878607	1.682479	-3.300000
H	-2.225776	-0.909505	-3.300000
H	-0.798527	-2.801627	-3.300000
H	1.687913	-2.458741	-3.300000

44 C U st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.221000	-0.448800	0.000000
N	-1.221000	0.968600	0.000000
C	-0.096454	1.723449	0.000000
C	1.127070	1.116940	0.000000
C	1.112692	-0.322388	0.000000
N	0.014110	-1.055259	0.000000
O	-2.294878	-1.037591	0.000000
N	2.297645	-0.991871	0.000000
H	-2.144657	1.393736	0.000000
H	-0.229047	2.806160	0.000000
H	2.047734	1.697075	0.000000
H	3.183948	-0.509430	0.000000
H	2.274439	-2.004205	0.000000
O	-0.229033	2.128032	3.300000
C	-0.314662	0.903502	3.300000
N	0.843848	0.104359	3.300000
C	0.945560	-1.277393	3.300000
N	-0.296049	-1.900498	3.300000
C	-1.494990	-1.223025	3.300000
C	-1.548033	0.127634	3.300000
O	2.004019	-1.891900	3.300000
H	1.729139	0.604967	3.300000
H	-0.265553	-2.913089	3.300000
H	-2.382508	-1.847430	3.300000
H	-2.490055	0.660236	3.300000

45 U PHE st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.825769	1.236525	-0.040250
C	1.300160	-0.062941	0.127256
C	0.403523	-1.128552	0.198245
C	-0.967809	-0.895190	0.103140
C	-1.443508	0.404483	-0.062441
C	-0.545755	1.468769	-0.136247
H	1.521013	2.063125	-0.082471
H	2.363658	-0.242261	0.207674
H	0.773753	-2.137427	0.324121
H	-1.665209	-1.719983	0.160427
H	-2.507511	0.585501	-0.124150
H	-0.914222	2.477422	-0.267855
N	-0.274881	0.671587	3.218646
C	1.117266	0.598601	3.350659

O	1.808176	1.593024	3.205825
C	1.596166	-0.735477	3.668769
C	0.716457	-1.749858	3.794986
N	-0.628789	-1.564826	3.624894
C	-1.203237	-0.340025	3.325479
O	-2.401026	-0.189202	3.183367
H	-0.648188	1.573349	2.955753
H	2.653218	-0.887693	3.802890
H	1.022384	-2.758279	4.031510
H	-1.277537	-2.327385	3.723763

46 T PHE st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	1.485450	-1.983330	-0.964780
C	0.278240	-1.983330	-1.667390
C	-0.933870	-1.983330	-0.973210
C	-0.938740	-1.983330	0.423570
C	0.268470	-1.983330	1.126190
C	1.480570	-1.983330	0.432010
H	2.429080	-1.983330	-1.505200
H	0.282030	-1.983330	-2.754810
H	-1.873700	-1.983330	-1.520230
H	-1.882380	-1.983330	0.963990
H	0.264680	-1.983330	2.213620
H	2.420410	-1.983330	0.979010
C	0.734360	1.516670	-0.488320
C	-0.619130	1.516670	-0.526610
C	-1.351710	1.516670	0.739040
N	-0.534300	1.516670	1.879030
C	0.849880	1.516670	1.951340
N	1.439100	1.516670	0.697420
O	1.485230	1.516670	2.998050
O	-2.576760	1.516670	0.844060
C	-1.416890	1.516670	-1.791480
H	1.339450	1.516670	-1.385040
H	-1.014580	1.516670	2.769740
H	2.446950	1.516670	0.701610
H	-0.764440	1.516670	-2.663150
H	-2.062650	0.640610	-1.835410
H	-2.062650	2.392730	-1.835410

47 A PHE st

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
C	0.705780	-1.926670	1.246410
C	1.402080	-1.926670	0.035530
C	0.701560	-1.926670	-1.172910
C	-0.695230	-1.926670	-1.170480
C	-1.391520	-1.926670	0.040400
C	-0.691010	-1.926670	1.248850
H	1.251150	-1.926670	2.187200
H	2.489510	-1.926670	0.033630
H	1.243640	-1.926670	-2.115610
H	-1.240590	-1.926670	-2.111270
H	-2.478950	-1.926670	0.042300
H	-1.233080	-1.926670	2.191540
C	1.046810	1.473330	0.052470
N	1.849740	1.473330	-1.067120
C	-0.254640	1.473330	-0.457810
N	-0.271250	1.473330	-1.838500
C	1.015870	1.473330	-2.156500
C	-1.292220	1.473330	0.496690
N	-0.975140	1.473330	1.801030
C	0.333930	1.473330	2.140050
N	1.411230	1.473330	1.345570
N	-2.595170	1.473330	0.133550
H	2.857500	1.473330	-1.069040
H	1.401880	1.473330	-3.163300
H	0.531370	1.473330	3.205460
H	-2.846430	1.473330	-0.838050
H	-3.300390	1.473330	0.847920

48 G PHE st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.525310	-1.974190	0.809020
C	1.234240	-1.974190	-0.394510
C	0.546420	-1.974190	-1.610230
C	-0.850330	-1.974190	-1.622410
C	-1.559250	-1.974190	-0.418890
C	-0.871430	-1.974190	0.796820
H	1.060780	-1.974190	1.755460
H	2.321630	-1.974190	-0.385020
H	1.098330	-1.974190	-2.547190
H	-1.385800	-1.974190	-2.568870
H	-2.646640	-1.974190	-0.428380
H	-1.423350	-1.974190	1.733780
C	0.778930	1.425810	-0.288640

C	-0.520970	1.425810	-0.791440
N	-0.532990	1.425810	-2.169820
C	0.749050	1.425810	-2.495910
C	-1.623230	1.425810	0.135350
N	-1.110870	1.425810	1.471500
C	0.210020	1.425810	1.850330
N	1.214420	1.425810	1.003950
O	-2.834190	1.425810	-0.049720
N	0.465510	1.425810	3.189260
N	1.580290	1.425810	-1.399900
H	1.136460	1.425810	-3.501550
H	-1.839280	1.425810	2.173680
H	-0.258040	1.425810	3.881500
H	1.426730	1.425810	3.475730
H	2.588030	1.425810	-1.391860

49 C PHE st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.771020	-1.875000	-1.819600
C	-0.625680	-1.875000	-1.802520
C	-1.309250	-1.875000	-0.584420
C	-0.596120	-1.875000	0.616620
C	0.800580	-1.875000	0.599550
C	1.484150	-1.875000	-0.618550
H	1.303190	-1.875000	-2.767910
H	-1.180860	-1.875000	-2.737560
H	-2.396590	-1.875000	-0.571140
H	-1.128290	-1.875000	1.564930
H	1.355760	-1.875000	1.534590
H	2.571490	-1.875000	-0.631840
C	0.844160	1.625000	-0.685410
C	-0.513060	1.625000	-0.628450
C	-1.088070	1.625000	0.689610
N	-0.391160	1.625000	1.810300
C	0.987140	1.625000	1.761780
N	1.564080	1.625000	0.464850
O	1.731310	1.625000	2.736600
N	-2.440110	1.625000	0.812370
H	1.402040	1.625000	-1.611730
H	-1.114810	1.625000	-1.523590
H	2.573210	1.625000	0.451770
H	-3.049480	1.625000	0.017050
H	-2.826160	1.625000	1.740230

50 TRP PHE st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-0.021074	1.531861	-1.363935
C	-1.274679	0.974103	-1.607410
C	-1.378305	-0.225698	-2.308415
C	-0.228943	-0.866405	-2.768794
C	1.024788	-0.303517	-2.531241
C	1.129000	0.896679	-1.829983
H	0.060074	2.456563	-0.809396
H	-2.165100	1.465452	-1.240568
H	-2.350973	-0.661612	-2.492670
H	-0.310342	-1.795576	-3.317270
H	1.916585	-0.794084	-2.899394
H	2.100035	1.332676	-1.640042
C	-2.022067	0.425854	1.901355
C	-0.814942	1.074045	2.106698
C	0.370429	0.449285	1.684746
C	1.750862	0.803894	1.719400
C	2.445136	-0.231074	1.135331
N	1.564646	-1.213781	0.755538
C	0.286121	-0.826949	1.061875
C	-0.928467	-1.485312	0.860694
C	-2.079285	-0.841767	1.287644
H	-2.941765	0.895383	2.223905
H	-0.785153	2.044381	2.585609
H	2.187011	1.699828	2.127590
H	3.502879	-0.348534	0.969523
H	1.807574	-2.036696	0.233304
H	-0.972920	-2.455485	0.383401
H	-3.038997	-1.320385	1.146840

51 pyridine···pyridine st

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.572481	0.254549	-0.256481
C	0.969360	-0.903160	0.044526
C	-0.398158	-1.028819	0.280960
C	-1.195805	0.106558	0.195397
C	-0.587128	1.317412	-0.120105
C	0.788547	1.339706	-0.332241
H	1.613639	-1.772181	0.102345
H	-0.818425	-1.991737	0.533564
H	-2.260690	0.049539	0.373443

H	-1.161812	2.229500	-0.200463
H	1.288432	2.268794	-0.578527
N	-0.533723	-1.515862	3.844144
C	-1.466201	-0.555232	3.917995
C	-1.204198	0.795836	3.708615
C	0.095229	1.185078	3.398347
C	1.074788	0.202179	3.314986
C	0.712309	-1.122958	3.548179
H	-2.468991	-0.886187	4.160188
H	-2.002756	1.520342	3.786887
H	0.337214	2.224076	3.222476
H	2.097090	0.448925	3.066549
H	1.456169	-1.908513	3.491730

52 U pyridine st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	1.210755	0.028676	0.329711
C	0.611935	-1.158449	0.153452
C	-0.751314	-1.308650	-0.088834
C	-1.547868	-0.169940	-0.156467
C	-0.943622	1.070636	0.019823
C	0.427719	1.116109	0.257349
H	1.251478	-2.029523	0.219293
H	-1.170416	-2.296869	-0.213383
H	-2.611013	-0.245955	-0.338756
H	-1.518814	1.984500	-0.011644
H	0.924695	2.068052	0.397548
N	-0.713168	-0.283949	3.297523
C	-0.712913	1.113860	3.390534
O	-1.752796	1.742060	3.275684
C	0.606582	1.672942	3.618097
C	1.676456	0.854250	3.689617
N	1.558395	-0.503044	3.577063
C	0.357948	-1.150276	3.350681
O	0.265810	-2.355694	3.217102
H	-1.608057	-0.715813	3.112920
H	0.707898	2.740164	3.713966
H	2.680335	1.222914	3.838044
H	2.371830	-1.095231	3.568895

53 U HIS st

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
C	1.431430	1.904000	-0.806810
N	0.202500	1.904000	-1.424520
C	1.150220	1.904000	0.541520
C	-0.751120	1.904000	-0.446250
N	-0.209040	1.904000	0.762570
H	2.356910	1.904000	-1.363430
H	0.037300	1.904000	-2.422950
H	1.851450	1.904000	1.364870
H	-1.810310	1.904000	-0.666580
N	-0.492530	-1.496000	1.709410
C	-1.681890	-1.496000	1.015400
C	-1.716790	-1.496000	-0.335730
C	-0.472730	-1.496000	-1.094900
O	-0.370380	-1.496000	-2.318110
N	0.674570	-1.496000	-0.280100
C	0.757440	-1.496000	1.103300
O	1.807680	-1.496000	1.731620
H	-0.475310	-1.496000	2.722360
H	-2.577190	-1.496000	1.628750
H	-2.651860	-1.496000	-0.879930
H	1.566920	-1.496000	-0.767790

54 T HIS st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.088530	-2.125000	-0.472230
N	-0.379830	-2.125000	0.706560
C	-0.130350	-2.125000	-1.461660
C	0.948960	-2.125000	0.389250
N	1.136710	-2.125000	-0.922180
H	-2.168230	-2.125000	-0.496280
H	-0.773710	-2.125000	1.638790
H	-0.283110	-2.125000	-2.532320
H	1.726520	-2.125000	1.141470
C	1.068260	1.375000	-0.521380
C	-0.284350	1.375000	-0.583290
C	-1.038900	1.375000	0.669380
N	-0.241520	1.375000	1.823460
C	1.141180	1.375000	1.919920
N	1.752200	1.375000	0.676470
O	1.758180	1.375000	2.977560
O	-2.265600	1.375000	0.753000
C	-1.059920	1.375000	-1.861890
H	1.688910	1.375000	-1.407410

H	-0.737270	1.375000	2.705650
H	2.759830	1.375000	0.698250
H	-0.392360	1.375000	-2.722040
H	-1.704810	0.498940	-1.917090
H	-1.704810	2.251060	-1.917090

55 A HIS st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.463640	-2.003570	-0.115130
N	0.273650	-2.003570	1.046000
C	0.470080	-2.003570	-1.127680
C	1.594290	-2.003570	0.696310
N	1.749930	-2.003570	-0.619310
H	-1.543600	-2.003570	-0.112800
H	-0.097340	-2.003570	1.987570
H	0.291210	-2.003570	-2.194280
H	2.390000	-2.003570	1.429310
C	0.755940	1.296430	0.022230
N	1.558860	1.296430	-1.097360
C	-0.545510	1.296430	-0.488050
N	-0.562130	1.296430	-1.868750
C	0.725000	1.296430	-2.186740
C	-1.583090	1.296430	0.466450
N	-1.266020	1.296430	1.770780
C	0.043060	1.296430	2.109790
N	1.120370	1.296430	1.315320
N	-2.886040	1.296430	0.103310
H	2.566630	1.296430	-1.099280
H	1.111010	1.296430	-3.193540
H	0.240490	1.296430	3.175210
H	-3.137300	1.296430	-0.868300
H	-3.591260	1.296430	0.817670

56 G HIS st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.035150	-2.110340	0.234680
N	-0.970000	-2.110340	-1.139220
C	0.277590	-2.110340	0.651580
C	0.350410	-2.110340	-1.489790
N	1.137440	-2.110340	-0.424120
H	-1.974380	-2.110340	0.767720

H	-1.758760	-2.110340	-1.773280
H	0.650670	-2.110340	1.666690
H	0.678410	-2.110340	-2.520740
C	0.868700	1.289660	-0.337650
N	1.670060	1.289660	-1.448920
C	-0.431200	1.289660	-0.840450
N	-0.443220	1.289660	-2.218830
C	0.838820	1.289660	-2.544930
C	-1.533460	1.289660	0.086330
N	-1.021100	1.289660	1.422490
C	0.299790	1.289660	1.801320
N	1.304190	1.289660	0.954930
O	-2.744420	1.289660	-0.098740
N	0.555280	1.289660	3.140240
H	2.677800	1.289660	-1.440880
H	1.226230	1.289660	-3.550570
H	-1.749510	1.289660	2.124670
H	-0.168270	1.289660	3.832480
H	1.516500	1.289660	3.426720

57 C HIS st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.051620	-2.019230	0.320930
N	1.162980	-2.019230	0.966350
C	0.260100	-2.019230	-1.020670
C	2.138540	-2.019230	0.009980
N	1.624030	-2.019230	-1.210830
H	-0.989490	-2.019230	0.856390
H	1.305490	-2.019230	1.968290
H	-0.422260	-2.019230	-1.859720
H	3.192470	-2.019230	0.254280
C	0.317590	1.480770	-1.224620
C	-1.040410	1.480770	-1.191330
C	-1.638340	1.480770	0.116480
N	-0.961090	1.480770	1.249160
C	0.417840	1.480770	1.224700
N	1.017330	1.480770	-0.061960
O	1.144890	1.480770	2.212380
N	-2.992310	1.480770	0.215630
H	0.891560	1.480770	-2.141060
H	-1.626440	1.480770	-2.096840
H	2.026540	1.480770	-0.057430
H	-3.587710	1.480770	-0.590200
H	-3.394490	1.480770	1.136600

58 U TRP st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.884320	1.487500	-0.044560
C	1.746700	1.487500	-1.413050
C	0.565810	1.487500	0.509780
N	0.405470	1.487500	-1.736260
C	-0.346190	1.487500	-0.582310
C	0.050540	1.487500	1.820330
C	-1.735990	1.487500	-0.405380
C	-1.325170	1.487500	2.001330
C	-2.209890	1.487500	0.899900
H	2.821630	1.487500	0.496650
H	2.499550	1.487500	-2.191030
H	0.033120	1.487500	-2.676300
H	0.722260	1.487500	2.676770
H	-2.418720	1.487500	-1.252970
H	-1.734910	1.487500	3.008590
H	-3.282700	1.487500	1.077960
N	0.019950	-1.912500	1.098050
C	-1.157110	-1.912500	0.383400
C	-1.168440	-1.912500	-0.968140
C	0.088690	-1.912500	-1.705470
O	0.212360	-1.912500	-2.926720
N	1.221600	-1.912500	-0.870770
C	1.280300	-1.912500	0.513850
O	2.319420	-1.912500	1.160400
H	0.019490	-1.912500	2.111150
H	-2.062970	-1.912500	0.981030
H	-2.093870	-1.912500	-1.528580
H	2.122320	-1.912500	-1.342830

59 T TRP st

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.642300	-1.602860	1.385580
C	-0.842770	-1.602860	2.504700
C	-0.773650	-1.602860	0.249270
N	0.481720	-1.602860	2.118610
C	0.560500	-1.602860	0.743700
C	-0.977830	-1.602860	-1.144060
C	1.678580	-1.602860	-0.100520
C	0.126030	-1.602860	-1.984810

C	1.441140	-1.602860	-1.468720
H	-2.724640	-1.602860	1.381740
H	-1.109440	-1.602860	3.553940
H	1.272010	-1.602860	2.749320
H	-1.986340	-1.602860	-1.553420
H	2.692260	-1.602860	0.295690
H	-0.019000	-1.602860	-3.062510
H	2.283590	-1.602860	-2.156380
C	0.978020	1.697140	-0.934890
C	-0.375480	1.697140	-0.973180
C	-1.108060	1.697140	0.292470
N	-0.290660	1.697140	1.432450
C	1.093520	1.697140	1.504770
N	1.682750	1.697140	0.250840
O	1.728880	1.697140	2.551480
O	-2.333110	1.697140	0.397480
C	-1.173230	1.697140	-2.238060
H	1.583100	1.697140	-1.831620
H	-0.770930	1.697140	2.323160
H	2.690600	1.697140	0.255020
H	-0.520800	1.697140	-3.109730
H	-1.819000	0.821080	-2.281980
H	-1.819000	2.573200	-2.281980

60 A TRP st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.288760	-1.700000	-1.056140
C	2.856000	-1.700000	0.196830
C	0.870050	-1.700000	-0.874500
N	1.857730	-1.700000	1.149080
C	0.628720	-1.700000	0.527710
C	-0.233000	-1.700000	-1.749900
C	-0.662390	-1.700000	1.071650
C	-1.513970	-1.700000	-1.216550
C	-1.727010	-1.700000	0.180050
H	2.828260	-1.700000	-1.994430
H	3.897500	-1.700000	0.492330
H	2.007040	-1.700000	2.149110
H	-0.081380	-1.700000	-2.827720
H	-0.827990	-1.700000	2.147320
H	-2.373610	-1.700000	-1.882500
H	-2.744450	-1.700000	0.564020
C	0.544080	1.800000	0.340880
N	1.347010	1.800000	-0.778720

C	-0.757360	1.800000	-0.169400
N	-0.773970	1.800000	-1.550110
C	0.513150	1.800000	-1.868100
C	-1.794950	1.800000	0.785090
N	-1.477860	1.800000	2.089420
C	-0.168780	1.800000	2.428440
N	0.908510	1.800000	1.633970
N	-3.097890	1.800000	0.421950
H	2.354780	1.800000	-0.780640
H	0.899150	1.800000	-2.874900
H	0.028650	1.800000	3.493860
H	-3.349150	1.800000	-0.549660
H	-3.803110	1.800000	1.136320

61 G TRP st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	1.250430	-1.700000	-0.972640
C	0.456760	-1.700000	-2.095930
C	0.375820	-1.700000	0.159100
N	-0.869740	-1.700000	-1.716790
C	-0.955710	-1.700000	-0.342310
C	0.572700	-1.700000	1.553480
C	-2.078210	-1.700000	0.496050
C	-0.535530	-1.700000	2.388440
C	-1.847930	-1.700000	1.865480
H	2.332720	-1.700000	-0.963140
H	0.728920	-1.700000	-3.143770
H	-1.656710	-1.700000	-2.351610
H	1.579070	-1.700000	1.968120
H	-3.089790	-1.700000	0.094550
H	-0.396150	-1.700000	3.466880
H	-2.693970	-1.700000	2.548720
C	1.026800	1.700000	-0.760520
C	-0.273100	1.700000	-1.263330
N	-0.285120	1.700000	-2.641710
C	0.996920	1.700000	-2.967810
C	-1.375360	1.700000	-0.336540
N	-0.863000	1.700000	0.999620
C	0.457890	1.700000	1.378440
N	1.462290	1.700000	0.532060
O	-2.586320	1.700000	-0.521620
N	0.713380	1.700000	2.717370
N	1.828160	1.700000	-1.871790
H	1.384330	1.700000	-3.973440

H	-1.591410	1.700000	1.701790
H	-0.010170	1.700000	3.409600
H	1.674600	1.700000	3.003830
H	2.835900	1.700000	-1.863750

62 C TRP st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.539990	-1.545450	0.875990
C	-0.722980	-1.545450	1.982410
C	-0.689280	-1.545450	-0.273820
N	0.595290	-1.545450	1.575570
C	0.652460	-1.545450	0.199600
C	-0.915320	-1.545450	-1.663780
C	1.757150	-1.545450	-0.662090
C	0.175190	-1.545450	-2.521760
C	1.498240	-1.545450	-2.026390
H	-2.622250	-1.545450	0.889160
H	-0.973130	-1.545450	3.035720
H	1.395380	-1.545450	2.193780
H	-1.930150	-1.545450	-2.057240
H	2.776920	-1.545450	-0.281860
H	0.013250	-1.545450	-3.597040
H	2.329780	-1.545450	-2.727200
C	0.858490	1.854550	-0.836630
C	-0.498730	1.854550	-0.779660
C	-1.073730	1.854550	0.538400
N	-0.376830	1.854550	1.659080
C	1.001470	1.854550	1.610560
N	1.578410	1.854550	0.313640
O	1.745650	1.854550	2.585390
N	-2.425780	1.854550	0.661160
H	1.416370	1.854550	-1.762940
H	-1.100470	1.854550	-1.674790
H	2.587540	1.854550	0.300560
H	-3.035140	1.854550	-0.134160
H	-2.811820	1.854550	1.589020

63 benzene dimer (C_{2V})

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.000000	0.000000	1.059035
C	0.000000	-1.206008	1.757674
C	0.000000	-1.207177	3.151591

C	0.000000	0.000000	3.848575
C	0.000000	1.207177	3.151591
C	0.000000	1.206008	1.757674
H	0.000000	0.000000	-0.021580
H	0.000000	-2.141639	1.214422
H	0.000000	-2.143566	3.692995
H	0.000000	0.000000	4.930150
H	0.000000	2.143566	3.692995
H	0.000000	2.141639	1.214422
C	-1.394063	0.000000	-2.454152
C	-0.697047	1.207238	-2.454628
C	0.697047	1.207238	-2.454628
C	1.394063	0.000000	-2.454152
C	0.697047	-1.207238	-2.454628
C	-0.697047	-1.207238	-2.454628
H	-2.475399	0.000000	-2.450322
H	-1.238232	2.143565	-2.453676
H	1.238232	2.143565	-2.453676
H	2.475399	0.000000	-2.450322
H	1.238232	-2.143565	-2.453676
H	-1.238232	-2.143565	-2.453676

64 U PHE edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-1.659130	-2.450000	-0.608720
C	-0.947050	-2.450000	-1.787100
C	0.404590	-2.450000	-1.801320
C	1.144460	-2.450000	-0.546080
O	2.365790	-2.450000	-0.423880
N	0.311810	-2.450000	0.589210
C	-1.072080	-2.450000	0.650940
O	-1.717210	-2.450000	1.690990
H	-2.672140	-2.450000	-0.607360
H	-1.545670	-2.450000	-2.692350
H	0.963280	-2.450000	-2.727810
H	0.786980	-2.450000	1.488450
C	-0.252410	1.240290	1.115080
C	0.956130	1.240370	0.414510
C	1.560300	2.450010	0.064290
C	0.956000	3.659750	0.414600
C	-0.252390	3.659660	1.115070
C	-0.856620	2.449900	1.465330
H	-0.722430	0.299020	1.387550
H	1.426190	0.299120	0.142030

H	2.500550	2.450210	-0.480750
H	1.426230	4.600880	0.142010
H	-0.722620	4.600800	1.387660
H	-1.796880	2.449980	2.010380

65 U PHE face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.278590	1.031680	-0.106450
C	0.741050	1.745390	-0.695140
C	0.751740	3.097050	-0.701310
C	-0.336230	3.835170	-0.073170
O	-0.443530	5.056330	-0.011220
N	-1.318420	3.000930	0.493900
C	-1.370210	1.616960	0.523790
O	-2.270130	0.970380	1.043370
H	-0.278540	0.018660	-0.106480
H	1.525750	1.148040	-1.148180
H	1.553420	3.657040	-1.164160
H	-2.097750	3.474840	0.943850
C	1.618270	-2.284830	-0.106470
C	0.919760	-2.284830	-1.316180
C	-0.476990	-2.284830	-1.316140
C	-1.175410	-2.284830	-0.106360
C	-0.476970	-2.284830	1.103210
C	0.919930	-2.284830	1.103180
H	2.705090	-2.284830	-0.106600
H	1.463240	-2.284830	-2.257340
H	-1.020560	-2.284830	-2.257230
H	-2.262220	-2.284830	-0.106500
H	-1.020250	-2.284830	2.044490
H	1.463260	-2.284830	2.044420

66 T PHE edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	0.135950	2.212900	-1.947820
C	-1.054520	2.212900	-1.249370
C	-1.100760	2.212900	0.104220
C	-2.369910	2.212900	0.897060
C	0.161270	2.212900	0.843140
O	0.259980	2.212900	2.069310
N	1.306420	2.212900	0.032770

C	1.386510	2.212900	-1.351310
O	2.437250	2.212900	-1.980620
H	0.146280	2.212900	-2.960800
H	-1.950860	2.212900	-1.863200
H	-3.242530	2.212900	0.238410
H	-2.417200	3.091960	1.545810
H	-2.417200	1.333850	1.545810
H	2.198240	2.212900	0.521690
C	0.165540	-3.896810	-0.479630
C	0.150910	-3.896720	0.917190
C	0.143600	-2.687090	1.615490
C	0.150910	-1.477340	0.917040
C	0.165540	-1.477430	-0.479620
C	0.172850	-2.687190	-1.178010
H	0.171230	-4.838080	-1.022890
H	0.145220	-4.837980	1.460490
H	0.132220	-2.686890	2.702230
H	0.145220	-0.536220	1.460530
H	0.171230	-0.536300	-1.023120
H	0.184230	-2.687120	-2.264760

67 T PHE face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.026680	0.612670	-0.441260
C	-1.052530	1.323130	0.148620
C	-1.080720	2.677120	0.164830
C	-2.173940	3.482770	0.793460
C	0.019750	3.403230	-0.467970
O	0.116070	4.628340	-0.523350
N	1.005330	2.581310	-1.034700
C	1.062590	1.196490	-1.067630
O	1.967920	0.556570	-1.588200
H	-0.026610	-0.400370	-0.441300
H	-1.834900	0.718410	0.598500
H	-2.936150	2.832980	1.231750
H	-1.771030	4.131960	1.575800
H	-2.647440	4.131960	0.051710
H	1.782680	3.061170	-1.481700
C	1.870190	-2.703850	0.061140
C	1.173780	-2.703850	-1.149780
C	-0.222970	-2.703850	-1.152180
C	-0.923500	-2.703850	0.056380
C	-0.227170	-2.703850	1.267170
C	1.169730	-2.703850	1.269570

H	2.957000	-2.703850	0.062910
H	1.718910	-2.703850	-2.089990
H	-0.764890	-2.703850	-2.094220
H	-2.010290	-2.703850	0.054350
H	-0.772080	-2.703850	2.207490
H	1.711430	-2.703850	2.211760

68 A PHE edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.052480	2.123330	1.046810
N	1.067120	2.123330	1.849740
C	0.457810	2.123330	-0.254640
N	1.838510	2.123330	-0.271250
C	2.156500	2.123330	1.015870
C	-0.496690	2.123330	-1.292220
N	-1.801020	2.123330	-0.975140
C	-2.140040	2.123330	0.333940
N	-1.345560	2.123330	1.411240
N	-0.133550	2.123330	-2.595170
H	1.069040	2.123330	2.857500
H	3.163300	2.123330	1.401880
H	-3.205460	2.123330	0.531370
H	0.838060	2.123330	-2.846430
H	-0.847920	2.123330	-3.300390
C	-1.434770	-2.776670	0.007710
C	-0.736370	-1.567000	0.006490
C	0.660430	-1.567010	0.004060
C	1.358830	-2.776670	0.002830
C	0.660430	-3.986330	0.004060
C	-0.736360	-3.986340	0.006500
H	-2.522210	-2.776670	0.009610
H	-1.280080	-0.625260	0.007450
H	1.204150	-0.625260	0.003110
H	2.446250	-2.776660	0.000940
H	1.204140	-4.928080	0.003110
H	-1.280080	-4.928080	0.007450

69 A PHE face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.194650	-2.623250	-1.306430
C	-1.893040	-2.623250	-0.096780

C	-1.194640	-2.623250	1.112880
C	0.202150	-2.623250	1.112880
C	0.900550	-2.623250	-0.096770
C	0.202150	-2.623250	-1.306440
H	-1.738370	-2.623250	-2.248180
H	-2.980480	-2.623250	-0.096780
H	-1.738360	-2.623250	2.054640
H	0.745870	-2.623250	2.054630
H	1.987990	-2.623250	-0.096770
H	0.745870	-2.623250	-2.248190
N	2.366460	3.411010	-0.096780
C	2.707990	2.102590	-0.096770
N	1.915580	1.023770	-0.096780
C	0.621790	1.385710	-0.096770
C	0.109020	2.686180	-0.096780
C	1.061520	3.725590	-0.096770
N	0.695870	5.027840	-0.096770
N	-1.271710	2.700140	-0.096770
C	-1.587230	1.412410	-0.096770
N	-0.496250	0.580640	-0.096770
H	3.773780	1.907200	-0.096780
H	-0.276210	5.277230	-0.096770
H	1.408890	5.734430	-0.096770
H	-2.593300	1.024470	-0.096780
H	-0.496240	-0.427130	-0.096770

70 G PHE edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.297830	2.143750	-1.785680
C	-2.384260	2.143750	-0.941960
N	-2.043010	2.143750	0.336530
C	-0.664890	2.143750	0.308820
C	0.275120	2.143750	1.399640
O	0.104370	2.143750	2.613160
N	1.605460	2.143750	0.872030
C	1.969050	2.143750	-0.453720
N	3.305040	2.143750	-0.726590
N	1.110180	2.143750	-1.447860
C	-0.177160	2.143750	-0.997090
H	-1.300200	2.143750	-2.798890
H	-3.399580	2.143750	-1.316830
H	2.317350	2.143750	1.598100
H	4.012590	2.143750	-0.010470
H	3.582420	2.143750	-1.696080

C	-0.632170	-3.965960	1.044880
C	0.064170	-3.965880	-0.166100
C	0.412290	-2.756240	-0.771480
C	0.064100	-1.546500	-0.165970
C	-0.637420	-1.546580	1.041800
C	-0.980310	-2.756350	1.650320
H	-0.902980	-4.907230	1.515840
H	0.335010	-4.907130	-0.637100
H	0.954040	-2.756050	-1.713620
H	0.335040	-0.605370	-0.637140
H	-0.903100	-0.605450	1.516050
H	-1.522070	-2.756270	2.592480

71 G PHE face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	1.686150	3.326950	-1.085240
C	0.533000	3.851530	-0.419470
O	0.382750	5.064670	-0.332720
C	-0.278920	2.758590	0.049290
C	0.146040	1.453780	-0.196060
N	1.261780	1.005940	-0.840230
C	2.003630	2.002020	-1.268540
N	3.161160	1.732190	-1.936840
N	-1.472460	2.783170	0.738380
C	-1.765480	1.503900	0.907560
N	-0.822950	0.662640	0.363390
H	2.301230	4.054630	-1.440360
H	3.772520	2.449900	-2.289810
H	3.403290	0.763330	-2.076630
H	-2.644040	1.126730	1.414790
H	-0.823000	-0.350560	0.363420
C	-0.124550	-2.653960	1.573090
C	0.573830	-2.653960	0.363300
C	-0.124580	-2.653960	-0.846290
C	-1.521490	-2.653960	-0.846260
C	-2.219780	-2.653960	0.363400
C	-1.521310	-2.653960	1.573130
H	0.418970	-2.653960	2.514230
H	1.660640	-2.653960	0.363400
H	0.418650	-2.653960	-1.787590
H	-2.064770	-2.653960	-1.787520
H	-3.306590	-2.653960	0.363540
H	-2.064780	-2.653960	2.514300

72 C PHE edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	1.489090	-2.365520	0.507200
C	0.747070	-2.365520	1.644450
C	-0.609210	-2.365520	1.562110
C	-1.159420	-2.365520	0.233190
N	-2.509110	-2.365520	0.083220
N	-0.440970	-2.365520	-0.874660
C	0.935890	-2.365520	-0.800240
O	1.698270	-2.365520	-1.761570
H	2.502910	-2.365520	0.537950
H	1.289850	-2.365520	2.585010
H	-1.230160	-2.365520	2.449880
H	-2.879700	-2.365520	-0.856770
H	-3.140690	-2.365520	0.867940
C	0.040830	1.324770	-1.152210
C	-0.000610	1.324850	0.244070
C	-0.021320	2.534490	0.942110
C	-0.000610	3.744230	0.243930
C	0.040830	3.744150	-1.152200
C	0.061550	2.534380	-1.850310
H	0.056950	0.383500	-1.695260
H	-0.016730	0.383600	0.787160
H	-0.053570	2.534680	2.028430
H	-0.016730	4.685360	0.787210
H	0.056960	4.685270	-1.695490
H	0.093790	2.534460	-2.936640

73 C PHE face

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.294440	0.762170	-0.087710
C	0.707480	1.469320	-0.670840
C	0.671940	2.827470	-0.650160
C	-0.461640	3.417770	0.009590
N	-0.555780	4.771400	0.064390
N	-1.437550	2.733290	0.577600
C	-1.409390	1.354810	0.561200
O	-2.259860	0.621970	1.056190
H	-0.294480	-0.252120	-0.087680
H	1.505750	0.898210	-1.135460
H	1.455150	3.421180	-1.106000
H	-1.358090	5.170360	0.531350

H	0.138690	5.378860	-0.339810
C	0.899730	-2.544980	-1.299840
C	-0.497160	-2.544980	-1.294880
C	-1.191270	-2.544980	-0.082810
C	-0.488560	-2.544980	1.124480
C	0.908160	-2.544980	1.119520
C	1.602360	-2.544980	-0.092670
H	1.439730	-2.544980	-2.243000
H	-1.043770	-2.544980	-2.234230
H	-2.278060	-2.544980	-0.078820
H	-1.028790	-2.544980	2.067500
H	1.454980	-2.544980	2.058750
H	2.689170	-2.544980	-0.096390

74 TRP PHE TS

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.511900	1.625015	0.000000
C	2.713009	0.957854	-1.208292
C	3.117782	-0.376744	-1.208365
C	3.321385	-1.043731	0.000000
C	3.117782	-0.376744	1.208365
C	2.713009	0.957854	1.208292
H	2.202404	2.661136	0.000000
H	2.551176	1.473691	-2.144590
H	3.270300	-0.895141	-2.144838
H	3.636814	-2.078152	0.000000
H	3.270300	-0.895141	2.144838
H	2.551176	1.473691	2.144590
N	-0.144241	-0.768693	0.000000
C	-0.516112	-2.089322	0.000000
C	-1.889876	-2.181449	0.000000
C	-2.393232	-0.847083	0.000000
C	-1.264065	0.019589	0.000000
C	-1.389600	1.411767	0.000000
C	-2.672650	1.936645	0.000000
C	-3.805451	1.097479	0.000000
C	-3.679817	-0.281721	0.000000
H	0.806524	-0.435887	0.000000
H	0.231002	-2.865317	0.000000
H	-2.458576	-3.095605	0.000000
H	-0.518873	2.053952	0.000000
H	-2.807757	3.009786	0.000000
H	-4.790599	1.543937	0.000000
H	-4.558019	-0.914292	0.000000

75 U HIS edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.958400	-1.960280	-0.036750
C	-1.260780	-1.960280	-1.223750
C	0.090590	-1.960280	-1.254480
C	0.845740	-1.960280	-0.008360
O	2.068470	-1.960280	0.098890
N	0.027020	-1.960280	1.137020
C	-1.356010	-1.960280	1.215640
O	-1.988390	-1.960280	2.263490
H	-2.971320	-1.960280	-0.023020
H	-1.870410	-1.960280	-2.121610
H	0.637930	-1.960280	-2.187720
H	0.513140	-1.960280	2.030370
C	0.504730	3.523030	0.319040
N	1.619690	2.717570	0.303460
C	-0.561660	2.651440	0.333920
C	1.191760	1.420350	0.309450
N	-0.130730	1.343470	0.327890
H	0.571870	4.600890	0.318090
H	2.581540	3.032010	0.290020
H	-1.615620	2.893500	0.348630
H	1.875740	0.582190	0.299900

76 U HIS face

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.609480	0.746070	-0.201840
C	-1.214110	1.459790	-1.212110
C	-1.220460	2.811450	-1.222690
C	-0.575310	3.549570	-0.144730
O	-0.511680	4.770720	-0.038420
N	0.007110	2.715330	0.828440
C	0.037820	1.331360	0.879740
O	0.571450	0.684770	1.771400
H	-0.609510	-0.266940	-0.201890
H	-1.679430	0.862440	-1.989590
H	-1.695840	3.371440	-2.017020
H	0.469240	3.189240	1.600600
C	1.567900	-2.570440	0.168980
N	0.836690	-2.570440	1.334090
C	0.628770	-2.570440	-0.838550

C	-0.485620	-2.570440	0.991400
N	-0.648380	-2.570440	-0.323410
H	2.647850	-2.570440	0.165860
H	1.213040	-2.570440	2.273540
H	0.801750	-2.570440	-1.906130
H	-1.277520	-2.570440	1.728530

77 T HIS edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	0.438990	1.750250	-2.154400
C	-0.751490	1.750250	-1.455950
C	-0.797720	1.750250	-0.102360
C	-2.066890	1.750250	0.690490
C	0.464300	1.750250	0.636560
O	0.563010	1.750250	1.862740
N	1.609450	1.750250	-0.173810
C	1.689540	1.750250	-1.557880
O	2.740290	1.750250	-2.187200
H	0.449320	1.750250	-3.167380
H	-1.647830	1.750250	-2.069770
H	-2.939500	1.750250	0.031830
H	-2.114160	2.629300	1.339240
H	-2.114160	0.871190	1.339240
H	2.501280	1.750250	0.315110
C	0.461810	-3.733060	0.459880
N	0.450130	-2.927600	1.574880
C	0.472980	-2.861470	-0.606560
C	0.454610	-1.630380	1.146930
N	0.468470	-1.553510	-0.175610
H	0.461110	-4.810920	0.527010
H	0.440060	-3.242040	2.536770
H	0.484010	-3.103530	-1.660560
H	0.447460	-0.792220	1.830940

78 T HIS face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.000240	0.312240	-0.009140
C	-0.593700	1.022700	-1.032920
C	-0.610020	2.376690	-1.061060
C	-1.242460	3.182340	-2.152080
C	0.026620	3.102790	0.037190

O	0.083070	4.327900	0.132900
N	0.596790	2.280880	1.020770
C	0.629920	0.896060	1.077930
O	1.153670	0.256140	1.981440
H	-0.000200	-0.700800	-0.009080
H	-1.046320	0.417980	-1.813730
H	-1.683400	2.532550	-2.912750
H	-2.023390	3.831530	-1.746450
H	-0.502370	3.831530	-2.628160
H	1.046500	2.760740	1.796570
C	1.678060	-3.004280	0.369950
N	0.938730	-3.004280	1.529930
C	0.745980	-3.004280	-0.644120
C	-0.381160	-3.004280	1.178020
N	-0.534730	-3.004280	-0.137900
H	2.758000	-3.004280	0.374360
H	1.308510	-3.004280	2.471980
H	0.926410	-3.004280	-1.710450
H	-1.178180	-3.004280	1.909600

79 A HIS edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.014880	1.611990	1.232450
N	1.134480	1.611990	2.035380
C	0.525160	1.611990	-0.069000
N	1.905870	1.611990	-0.085610
C	2.223860	1.611990	1.201510
C	-0.429330	1.611990	-1.106580
N	-1.733660	1.611990	-0.789500
C	-2.072680	1.611990	0.519580
N	-1.278200	1.611990	1.596880
N	-0.066190	1.611990	-2.409530
H	1.136400	1.611990	3.043150
H	3.230670	1.611990	1.587520
H	-3.138100	1.611990	0.717010
H	0.905420	1.611990	-2.660790
H	-0.780560	1.611990	-3.114740
C	-1.086020	-3.186380	-0.307120
N	-0.644720	-1.883670	-0.307890
C	0.060950	-3.948980	-0.309130
C	0.721170	-1.910630	-0.310270
N	1.183980	-3.151960	-0.311090
H	-2.135810	-3.439890	-0.305300
H	-1.228140	-1.056750	-0.306870

H	0.139780	-5.027600	-0.309270
H	1.320640	-1.010030	-0.311330

80 A HIS face

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.515190	-2.862790	-0.339390
N	0.735850	-2.862790	0.793940
C	0.619190	-2.862790	-1.385470
C	-0.571100	-2.862790	0.396100
N	-0.678430	-2.862790	-0.924340
H	2.594340	-2.862790	-0.297480
H	1.072080	-2.862790	1.748480
H	0.837030	-2.862790	-2.444800
H	-1.393130	-2.862790	1.099450
N	0.668570	3.271470	1.772520
C	0.827850	1.963050	2.074620
N	0.458290	0.884230	1.373680
C	-0.145120	1.246170	0.229210
C	-0.384270	2.546640	-0.224380
C	0.059970	3.586050	0.618200
N	-0.110570	4.888300	0.294740
N	-1.028230	2.560600	-1.445750
C	-1.175380	1.272870	-1.724850
N	-0.666550	0.441090	-0.759790
H	1.324930	1.767660	3.017400
H	-0.563930	5.137690	-0.565140
H	0.221970	5.594880	0.925470
H	-1.644600	0.884930	-2.614790
H	-0.666550	-0.566680	-0.759780

81 G HIS edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.531020	1.653460	1.322610
C	-0.685390	1.653460	2.407570
N	0.592510	1.653460	2.064090
C	0.562390	1.653460	0.686030
C	1.651560	1.653460	-0.255890
O	2.865390	1.653460	-0.087260
N	1.121640	1.653460	-1.585300
C	-0.204750	1.653460	-1.946570
N	-0.479940	1.653460	-3.282090

N	-1.197380	1.653460	-1.085980
C	-0.744370	1.653460	0.200570
H	-2.544210	1.653460	1.326750
H	-1.058480	1.653460	3.423550
H	1.846460	1.653460	-2.298460
H	0.234930	1.653460	-3.990900
H	-1.449910	1.653460	-3.557780
C	0.749760	-3.160190	1.265040
N	0.536720	-1.851450	0.899000
C	0.167600	-3.906960	0.264780
C	-0.150390	-1.859760	-0.281580
N	-0.391780	-3.094650	-0.696330
H	1.276060	-3.427770	2.169310
H	0.836030	-1.032830	1.413250
H	0.120400	-4.984390	0.183700
H	-0.445760	-0.951120	-0.789070

82 G HIS face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	0.196590	-3.042600	-1.169670
C	0.866380	-3.567180	-0.018860
O	0.953660	-4.780310	0.131090
C	1.337980	-2.474230	0.791430
C	1.091150	-1.169430	0.367330
N	0.443080	-0.721580	-0.746160
C	0.012190	-1.717660	-1.486510
N	-0.660140	-1.447830	-2.641700
N	2.031230	-2.498820	1.982560
C	2.201430	-1.219550	2.274980
N	1.653970	-0.378290	1.334350
H	-0.160670	-3.770270	-1.783510
H	-1.015250	-2.165550	-3.251810
H	-0.800790	-0.478980	-2.883340
H	2.711730	-0.842380	3.151760
H	1.654000	0.634920	1.334410
C	-0.523180	2.938310	0.965590
N	0.205990	2.938310	-0.200790
C	0.417700	2.938310	1.971480
C	1.528900	2.938310	0.139580
N	1.693950	2.938310	1.454110
H	-1.603130	2.938310	0.970600
H	-0.172000	2.938310	-1.139580
H	0.246590	2.938310	3.039360
H	2.319510	2.938310	-0.598920

83 C HIS edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.696340	-1.843220	-1.594130
C	1.855110	-1.843220	-0.886170
C	1.813040	-1.843220	0.471950
C	0.501040	-1.843220	1.061340
N	0.391170	-1.843220	2.414890
N	-0.627650	-1.843220	0.376080
C	-0.594110	-1.843220	-1.002380
O	-1.577630	-1.843220	-1.735910
H	0.697010	-1.843220	-2.608420
H	2.779150	-1.843220	-1.456630
H	2.718840	-1.843220	1.066300
H	-0.537420	-1.843220	2.813210
H	1.194260	-1.843220	3.022910
C	-1.836690	2.955090	-0.612100
N	-1.395180	1.652320	-0.612110
C	-0.689760	3.717750	-0.612110
C	-0.029450	1.679470	-0.612100
N	0.433370	2.920850	-0.612100
H	-2.886550	3.208220	-0.612110
H	-1.978840	0.825580	-0.612110
H	-0.610810	4.796380	-0.612110
H	0.570220	0.779000	-0.612100

84 C HIS face

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.369020	0.460770	0.032490
C	-0.948650	1.167920	-0.971460
C	-0.928090	2.526070	-0.935840
C	-0.272300	3.116370	0.200030
N	-0.217830	4.470000	0.294360
N	0.292290	2.431900	1.177910
C	0.276000	1.053420	1.149700
O	0.768020	0.320570	2.001900
H	-0.369000	-0.553520	0.032530
H	-1.410480	0.596820	-1.771360
H	-1.381190	3.119780	-1.720650
H	0.246320	4.868960	1.098300
H	-0.619600	5.077460	-0.401520
C	1.309270	-2.856380	-0.088410

N	0.569930	-2.856380	1.071560
C	0.377190	-2.856380	-1.102480
C	-0.749950	-2.856380	0.719650
N	-0.903530	-2.856380	-0.596270
H	2.389200	-2.856380	-0.084000
H	0.939720	-2.856380	2.013610
H	0.557620	-2.856380	-2.168820
H	-1.546980	-2.856380	1.451220

85 U TRP edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-2.296070	-2.822930	-0.101380
C	-1.577840	-2.822930	-1.276010
C	-0.226140	-2.822930	-1.283160
C	0.507150	-2.822930	-0.024060
O	1.727820	-2.822930	0.104520
N	-0.331440	-2.822930	1.106870
C	-1.715630	-2.822930	1.161340
O	-2.366200	-2.822930	2.198000
H	-3.309080	-2.822930	-0.105320
H	-2.171700	-2.822930	-2.184390
H	0.337390	-2.822930	-2.206700
H	0.139010	-2.822930	2.008570
C	2.488190	3.081390	-0.213740
C	3.070710	1.835450	-0.211700
C	1.071810	2.882380	-0.218680
N	2.084180	0.871050	-0.215160
C	0.847660	1.477330	-0.219470
C	-0.041870	3.744220	-0.222570
C	-0.436690	0.917640	-0.223950
C	-1.316210	3.195220	-0.227020
C	-1.512140	1.796130	-0.227710
H	3.016170	4.026200	-0.211900
H	4.115740	1.552730	-0.208060
H	2.245700	-0.127070	-0.214590
H	0.096540	4.823820	-0.222090
H	-0.589090	-0.159990	-0.224480
H	-2.183930	3.850600	-0.230050
H	-2.524780	1.399720	-0.231240

86 U TRP face

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
N	-0.552770	1.446840	-0.705540
C	0.626030	1.513230	0.002760
C	1.187440	2.695660	0.340090
C	0.542250	3.943250	-0.047580
O	0.947710	5.075880	0.196040
N	-0.653180	3.750300	-0.765870
C	-1.263560	2.562070	-1.132610
O	-2.310760	2.488830	-1.761830
H	-0.966510	0.556230	-0.954140
H	1.064830	0.556280	0.266420
H	2.113780	2.746840	0.896700
H	-1.137740	4.595780	-1.057010
C	-1.059340	-1.943750	-1.499330
C	-2.175700	-1.943750	-0.695920
C	0.079960	-1.943750	-0.634620
N	-1.785020	-1.943750	0.627220
C	-0.409840	-1.943750	0.701240
C	1.472590	-1.943750	-0.843620
C	0.438250	-1.943750	1.816390
C	2.317150	-1.943750	0.257320
C	1.805620	-1.943750	1.574200
H	-1.059300	-1.943750	-2.581670
H	-3.225850	-1.943750	-0.958950
H	-2.412950	-1.943750	1.419700
H	1.878450	-1.943750	-1.853550
H	0.045560	-1.943750	2.831430
H	3.394350	-1.943750	0.108550
H	2.496200	-1.943750	2.414270

87 T TRP edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	0.141130	2.529530	-2.200300
C	-1.058980	2.529530	-1.518540
C	-1.124110	2.529530	-0.165730
C	-2.404220	2.529530	0.609310
C	0.127480	2.529530	0.590740
O	0.209060	2.529530	1.818170
N	1.283830	2.529530	-0.203560
C	1.383230	2.529530	-1.586390
O	2.442670	2.529530	-2.200960
H	0.165610	2.529530	-3.213030
H	-1.946660	2.529530	-2.144830
H	-3.267550	2.529530	-0.061450

H	-2.460560	3.408590	1.257350
H	-2.460560	1.650480	1.257350
H	2.168740	2.529530	0.297760
C	0.096760	-3.274780	2.241150
C	0.082530	-2.028840	2.823510
C	0.131370	-3.075780	0.825190
N	0.106630	-1.064440	1.837260
C	0.136850	-1.670720	0.601100
C	0.158580	-3.937610	-0.288170
C	0.168230	-1.111030	-0.682860
C	0.189710	-3.388620	-1.562130
C	0.194500	-1.989520	-1.758000
H	0.083860	-4.219590	2.768990
H	0.057000	-1.746120	3.868230
H	0.102690	-0.066320	1.998750
H	0.155200	-5.017220	-0.149790
H	0.171950	-0.033400	-0.835220
H	0.210910	-4.044000	-2.429590
H	0.219240	-1.593120	-2.770350

88 T TRP face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.893420	1.196950	-0.698980
C	0.270600	1.263650	0.039720
C	0.835200	2.441430	0.398040
C	2.095040	2.555280	1.197550
C	0.180490	3.681370	-0.017450
O	0.586780	4.813480	0.240380
N	-0.993450	3.494490	-0.762450
C	-1.595310	2.305390	-1.144420
O	-2.627720	2.235140	-1.799610
H	-1.297790	0.304270	-0.955600
H	0.700740	0.304140	0.312710
H	2.489890	1.567050	1.448130
H	2.855450	3.108120	0.639000
H	1.913410	3.108120	2.123420
H	-1.469120	4.341240	-1.064320
C	-1.407020	-2.195790	-1.476920
C	-2.523370	-2.195790	-0.673510
C	-0.267710	-2.195790	-0.612210
N	-2.132690	-2.195790	0.649630
C	-0.757510	-2.195790	0.723650
C	1.124910	-2.195790	-0.821210
C	0.090580	-2.195790	1.838800

C	1.969470	-2.195790	0.279730
C	1.457950	-2.195790	1.596610
H	-1.406970	-2.195790	-2.559260
H	-3.573530	-2.195790	-0.936540
H	-2.760630	-2.195790	1.442100
H	1.530770	-2.195790	-1.831140
H	-0.302120	-2.195790	2.853840
H	3.046660	-2.195790	0.130950
H	2.148520	-2.195790	2.436680

89 A TRP edge

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.957870	2.529530	-0.228670
N	1.760800	2.529530	-1.348270
C	-0.343580	2.529530	-0.738950
N	-0.360200	2.529530	-2.119660
C	0.926930	2.529530	-2.437650
C	-1.381160	2.529530	0.215550
N	-1.064090	2.529530	1.519870
C	0.244990	2.529530	1.858890
N	1.322290	2.529530	1.064420
N	-2.684110	2.529530	-0.147600
H	2.768560	2.529530	-1.350190
H	1.312940	2.529530	-3.444450
H	0.442420	2.529530	2.924300
H	-2.935370	2.529530	-1.119210
H	-3.389330	2.529530	0.566770
C	-0.968630	-3.274730	1.795820
C	-1.259010	-2.028790	2.300790
C	-0.262570	-3.075760	0.567950
N	-0.767200	-1.064410	1.445540
C	-0.150820	-1.670720	0.373610
C	0.292560	-3.937630	-0.397480
C	0.489430	-1.111070	-0.739810
C	0.927810	-3.388670	-1.502220
C	1.025510	-1.989580	-1.672090
H	-1.231810	-4.219560	2.253520
H	-1.779930	-1.746040	3.206710
H	-0.847720	-0.066290	1.585560
H	0.223550	-5.017240	-0.277460
H	0.565410	-0.033440	-0.871950
H	1.360360	-4.044070	-2.254430
H	1.530320	-1.593200	-2.549970

90 A TRP face

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.973420	-2.258910	2.003000
C	2.084110	-2.258910	1.191790
C	-0.171920	-2.258910	1.146290
N	1.684180	-2.258910	-0.128580
C	0.308520	-2.258910	-0.192970
C	-1.563040	-2.258910	1.365040
C	-0.547370	-2.258910	-1.302140
C	-2.415300	-2.258910	0.270060
C	-1.913010	-2.258910	-1.050390
H	0.980920	-2.258910	3.085310
H	3.136090	-2.258910	1.447460
H	2.306560	-2.258910	-0.925430
H	-1.961810	-2.258910	2.377800
H	-0.161800	-2.258910	-2.319920
H	-3.491420	-2.258910	0.426360
H	-2.609460	-2.258910	-1.885590
N	1.822470	3.775350	-1.593290
C	2.117060	2.466930	-1.766120
N	1.433590	1.388110	-1.365130
C	0.317680	1.750050	-0.710430
C	-0.124590	3.050520	-0.450950
C	0.696950	4.089930	-0.932940
N	0.381580	5.392180	-0.747920
N	-1.315490	3.064480	0.247760
C	-1.587640	1.776750	0.407420
N	-0.646650	0.944980	-0.144670
H	3.036320	2.271540	-2.305440
H	-0.456860	5.641570	-0.256010
H	0.996560	6.098770	-1.108730
H	-2.455380	1.388810	0.916510
H	-0.646640	-0.062790	-0.144660

91 G TRP edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-1.722530	2.459270	1.191890
C	-0.878800	2.459270	2.278330
N	0.399690	2.459270	1.937070
C	0.371980	2.459270	0.558950
C	1.462800	2.459270	-0.381050
O	2.676320	2.459270	-0.210300

N	0.935190	2.459270	-1.711400
C	-0.390570	2.459270	-2.074980
N	-0.663430	2.459270	-3.410970
N	-1.384710	2.459270	-1.216110
C	-0.933930	2.459270	0.071220
H	-2.735730	2.459270	1.194260
H	-1.253680	2.459270	3.293650
H	1.661260	2.459270	-2.423280
H	-1.632920	2.459270	-3.688360
H	0.052680	2.459270	-4.118530
C	0.892890	-3.345040	2.213940
C	1.185040	-2.099110	2.717920
C	0.182560	-3.146040	0.988570
N	0.690270	-1.134700	1.864420
C	0.070150	-1.740990	0.794640
C	-0.375970	-4.007880	0.025040
C	-0.573970	-1.181300	-0.316520
C	-1.015060	-3.458880	-1.077450
C	-1.113330	-2.059780	-1.246960
H	1.157680	-4.289860	2.670740
H	1.709130	-1.816390	3.622040
H	0.771290	-0.136580	2.004170
H	-0.306550	-5.087480	0.144800
H	-0.650410	-0.103670	-0.448390
H	-1.450240	-4.114260	-1.828170
H	-1.621180	-1.663380	-2.123060

92 G TRP face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	0.400620	4.551690	-0.844900
C	-0.294920	4.215480	0.359810
O	-0.714600	5.108390	1.086720
C	-0.364340	2.782230	0.480060
C	0.211450	1.996660	-0.517250
N	0.867270	2.370840	-1.653180
C	0.931430	3.678310	-1.764290
N	1.555830	4.225880	-2.845780
N	-0.935260	2.010080	1.468910
C	-0.705980	0.768820	1.071790
N	-0.018910	0.706110	-0.118250
H	0.482050	5.555410	-0.985930
H	1.638340	5.218970	-2.988710
H	1.948690	3.593840	-3.526240
H	-1.012620	-0.122980	1.602910

H	0.272290	-0.122990	-0.622630
C	-2.013940	-2.722990	1.615900
C	-1.198880	-2.722990	2.723780
C	-1.161210	-2.722990	0.467610
N	0.120100	-2.722990	2.319260
C	0.179700	-2.722990	0.943390
C	-1.384780	-2.722990	-0.922750
C	1.285910	-2.722990	0.083670
C	-0.292750	-2.722990	-1.778800
C	1.029430	-2.722990	-1.281090
H	-3.096220	-2.722990	1.627190
H	-1.450910	-2.722990	3.776640
H	0.919110	-2.722990	2.938880
H	-2.398910	-2.722990	-1.318020
H	2.305010	-2.722990	0.465710
H	-0.452790	-2.722990	-2.854370
H	1.862210	-2.722990	-1.980430

93 C TRP edge

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.949500	-2.684870	-0.759370
C	-0.243570	-2.684870	-1.919370
C	1.114630	-2.684870	-1.879670
C	1.706300	-2.684870	-0.568700
N	3.060050	-2.684870	-0.461190
N	1.023010	-2.684870	0.561180
C	-0.355500	-2.684870	0.530050
O	-1.087320	-2.684870	1.514840
H	-1.963790	-2.684870	-0.758270
H	-0.815630	-2.684870	-2.842420
H	1.707390	-2.684870	-2.786510
H	3.459980	-2.684870	0.466700
H	3.666670	-2.684870	-1.265350
C	-0.463560	2.993400	2.489610
C	-0.462710	1.709860	2.983800
C	-0.466060	2.893690	1.062790
N	-0.464530	0.816620	1.932400
C	-0.466610	1.507690	0.741170
C	-0.467890	3.831110	0.011940
C	-0.468920	1.038950	-0.579090
C	-0.470170	3.372340	-1.297600
C	-0.470690	1.990320	-1.590660
H	-0.462540	3.899080	3.082210
H	-0.460920	1.354940	4.006570

H	-0.464380	-0.190330	2.023900
H	-0.467520	4.898430	0.225330
H	-0.469320	-0.025420	-0.806300
H	-0.471610	4.086660	-2.117490
H	-0.472480	1.665520	-2.628490

94 C TRP face

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	3.944973	0.254304	0.063512
C	4.009961	-0.951745	-0.557069
C	2.868819	-1.654091	-0.782430
C	1.650568	-1.038494	-0.328932
N	0.475294	-1.690132	-0.524591
N	1.583707	0.133930	0.274752
C	2.736822	0.853292	0.507388
O	2.790813	1.948472	1.057887
H	4.780029	0.800720	0.244926
H	4.995818	-1.301551	-0.848637
H	2.885934	-2.618936	-1.274873
H	-0.371431	-1.244294	-0.200257
H	0.423766	-2.589286	-0.975717
C	-2.414864	1.348468	-1.638455
C	-1.665133	2.314509	-1.008867
C	-2.611491	0.289972	-0.696840
N	-1.386106	1.907292	0.279411
C	-1.950693	0.671444	0.504095
C	-3.279065	-0.949324	-0.736310
C	-1.937955	-0.136816	1.648377
C	-3.269620	-1.753824	0.394206
C	-2.605907	-1.352060	1.574858
H	-2.780137	1.395074	-2.656225
H	-1.303672	3.267181	-1.374647
H	-0.849455	2.436013	0.953798
H	-3.793898	-1.269615	-1.640236
H	-1.427061	0.171426	2.558581
H	-3.781639	-2.712971	0.375792
H	-2.618475	-2.007266	2.442683

95 ethyne···ethyne (CH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.601730	-0.028570	0.384935
C	0.610109	-0.028664	0.388164

H	-1.663735	-0.028527	0.379014
H	1.672135	-0.028793	0.387968
C	-0.007360	0.100337	4.142812
C	-0.011296	0.138627	5.354277
H	-0.003966	0.066602	3.079515
H	-0.014563	0.172003	6.415189

96 PHE···ethyne (CH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.836612	1.114856	0.231008
C	1.384188	-0.166965	0.260057
C	0.547479	-1.281847	0.286931
C	-0.836667	-1.115004	0.284563
C	-1.384163	0.166850	0.255605
C	-0.547498	1.281748	0.228977
H	1.485452	1.979680	0.214705
H	2.457684	-0.296288	0.266060
H	0.971918	-2.275979	0.313877
H	-1.485554	-1.979569	0.309698
H	-2.457645	0.296459	0.258541
H	-0.972141	2.276001	0.211161
C	0.005855	0.075150	3.779452
C	0.009515	0.094731	4.991828
H	0.002846	0.057595	2.715376
H	0.012628	0.111904	6.053025

97 PHE···AcOH (OH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.964080	0.875093	0.378014
C	1.431057	-0.413133	0.118992
C	0.534128	-1.477639	0.042418
C	-0.830327	-1.253604	0.220856
C	-1.297587	0.034413	0.480243
C	-0.400445	1.099779	0.561601
H	1.659830	1.699931	0.446042
H	2.489525	-0.587209	-0.017013
H	0.896961	-2.477388	-0.152012
H	-1.525760	-2.079624	0.164117
H	-2.354396	0.208016	0.628561
H	-0.760455	2.093769	0.784757
C	-0.119855	0.534389	4.360081

O	-0.588045	1.583836	3.980821
O	0.283357	-0.443174	3.520796
C	0.090099	0.137402	5.791487
H	0.114653	-0.117260	2.619391
H	-0.219867	0.946739	6.441476
H	-0.485982	-0.759222	6.008438
H	1.138597	-0.098730	5.956506

98 PHE···$AcNH_2$ (NH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.855561	0.358532	1.049754
C	1.342897	-0.675379	0.251157
C	0.477807	-1.376701	-0.587816
C	-0.874830	-1.042556	-0.630452
C	-1.362397	-0.007014	0.165846
C	-0.498444	0.693157	1.006992
H	1.513826	0.902680	1.712766
H	2.392884	-0.933345	0.281963
H	0.856084	-2.178908	-1.206824
H	-1.545406	-1.585700	-1.282416
H	-2.411571	0.253467	0.130779
H	-0.866111	1.490340	1.638037
C	0.081929	0.497531	4.804729
O	0.328419	1.540957	4.217489
N	-0.222118	-0.657476	4.153561
C	0.104774	0.402639	6.313146
H	-0.196918	-0.664491	3.146925
H	-0.377894	-1.512968	4.649263
H	1.136488	0.486851	6.648220
H	-0.317130	-0.524004	6.694172
H	-0.444691	1.246485	6.719917

99 PHE···MeOH (OH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.759749	1.031275	0.373772
C	1.266618	-0.267362	0.421273
C	0.395321	-1.355991	0.424905
C	-0.982206	-1.146654	0.381270
C	-1.489346	0.151150	0.337572
C	-0.618775	1.240331	0.333884
H	1.435016	1.875664	0.374705

H	2.334916	-0.429180	0.459432
H	0.788662	-2.362493	0.463035
H	-1.657656	-1.991140	0.385121
H	-2.557947	0.313750	0.307719
H	-1.011762	2.247107	0.304369
O	0.047019	0.306185	3.685113
C	-0.849132	-0.751429	3.968168
H	0.133119	0.356058	2.727920
H	-0.944852	-0.808163	5.049104
H	-1.841281	-0.579731	3.544378
H	-0.482671	-1.714470	3.605257

100 PHE···peptide (NH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.408780	1.051025	0.375536
C	1.019168	-0.199770	0.289053
C	0.241723	-1.356883	0.296690
C	-1.146180	-1.264258	0.393902
C	-1.757278	-0.013960	0.482952
C	-0.979686	1.144207	0.472284
H	1.011939	1.948546	0.368078
H	2.095571	-0.271833	0.217191
H	0.715216	-2.326589	0.228072
H	-1.749182	-2.161927	0.399410
H	-2.833514	0.058244	0.559039
H	-1.454051	2.114001	0.537136
C	0.245622	1.956758	4.256635
C	0.208775	0.503594	4.672344
O	0.493404	0.151233	5.810882
N	-0.163620	-0.362122	3.693103
C	-0.200413	-1.789001	3.911190
H	-0.112523	2.122488	3.243343
H	1.270205	2.313467	4.338077
H	-0.358475	2.530393	4.954988
H	-0.324748	-0.004132	2.767035
H	-0.122325	-1.955909	4.981186
H	-1.135653	-2.207352	3.544452
H	0.628714	-2.292874	3.413853

101 ethyne···AcOH (OH···π)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

C	-0.610563	0.227503	-0.170602
C	-1.386276	-0.525326	0.379974
H	0.107385	0.861436	-0.634209
H	-2.080703	-1.174067	0.854379
C	2.834450	-0.641431	0.465936
O	2.580271	0.314671	-0.232902
O	1.886545	-1.415772	1.033623
C	4.210085	-1.122881	0.816087
H	1.025546	-1.048473	0.765851
H	4.948471	-0.485331	0.345237
H	4.336295	-1.111026	1.896122
H	4.332362	-2.150726	0.482853

102 PHE···AcOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.606785	1.330422	0.316435
C	1.118085	0.087249	0.685117
C	0.292902	-1.036087	0.669107
C	-1.042832	-0.916711	0.288190
C	-1.553588	0.327349	-0.079943
C	-0.728042	1.450843	-0.066848
H	1.246498	2.202264	0.330352
H	2.150058	-0.003887	0.993758
H	0.688497	-2.000961	0.955378
H	-1.682710	-1.788488	0.279349
H	-2.589235	0.420289	-0.377346
H	-1.123624	2.415659	-0.353861
C	0.418987	-0.271679	4.024977
O	1.614480	-0.107728	4.101493
O	-0.160515	-1.483084	4.224415
C	-0.602897	0.772253	3.704296
H	0.573936	-2.084192	4.417453
H	-0.124603	1.743199	3.657473
H	-1.055697	0.539056	2.741588
H	-1.387748	0.766716	4.456795

103 $MeNH_2$···pyridine

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.541059	0.029576	-0.208995
C	-0.078799	1.042390	0.738459
H	0.055553	-0.786118	-0.130293

H	-1.469669	-0.274708	0.053143
H	-0.720153	1.919414	0.671980
H	-0.050758	0.723823	1.785515
H	0.926431	1.356604	0.461999
N	2.341850	-1.256800	0.030153
C	2.680287	-0.444456	-0.981559
C	3.651616	0.547678	-0.881192
C	4.312456	0.717219	0.331072
C	3.972323	-0.117743	1.390195
C	2.988541	-1.082532	1.191012
H	2.137619	-0.588994	-1.906941
H	3.876468	1.172018	-1.734043
H	5.070310	1.479457	0.447456
H	4.454911	-0.027281	2.352896
H	2.702457	-1.746280	1.997622

104 peptide···ethene

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	1.629715	0.503013	0.270112
C	0.261828	-0.132861	0.314562
O	0.099253	-1.309616	0.611840
N	-0.773502	0.702512	0.022076
C	-2.150012	0.265969	0.095053
H	1.641573	1.459238	-0.248083
H	2.315319	-0.183555	-0.217586
H	1.969746	0.649360	1.293981
H	-0.569011	1.666557	-0.165814
H	-2.144738	-0.819407	0.100912
H	-2.640543	0.615820	1.003604
H	-2.707744	0.620751	-0.768261
C	-0.045756	0.517997	3.776217
C	0.722754	-0.568965	3.846026
H	-0.050638	1.260171	4.562099
H	-0.694289	0.685766	2.927533
H	1.368059	-0.740791	4.696154
H	0.717642	-1.304165	3.053717

105 PHE···cyclopentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.765545	0.868244	0.820991
C	1.237653	-0.442838	0.793888

C	0.372237	-1.488537	0.477269
C	-0.964933	-1.222972	0.186878
C	-1.437065	0.088406	0.213277
C	-0.571906	1.134024	0.530813
H	1.437476	1.680007	1.065103
H	2.275759	-0.648538	1.017711
H	0.738188	-2.506080	0.457056
H	-1.636459	-2.034561	-0.057774
H	-2.474684	0.294302	-0.011467
H	-0.937699	2.151711	0.551078
C	-0.763453	-0.726774	4.059828
C	0.706088	-0.983837	4.403958
C	1.346225	0.421560	4.494910
C	0.167179	1.420737	4.521782
C	-1.066593	0.563642	4.817431
H	-0.869707	-0.551825	2.987521
H	-1.415091	-1.556038	4.332978
H	1.201319	-1.621422	3.673373
H	0.769367	-1.484051	5.371424
H	1.996493	0.614231	3.643058
H	1.959092	0.510729	5.390636
H	0.050027	1.879707	3.539497
H	0.312773	2.222242	5.244181
H	-1.997581	1.039379	4.511518
H	-1.132019	0.354321	5.887967

106 PHE···neopentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.311954	0.561023	0.496699
C	1.142182	-0.558075	0.536062
C	0.587804	-1.836687	0.554144
C	-0.796658	-1.996376	0.532963
C	-1.626893	-0.877474	0.494168
C	-1.072665	0.401206	0.475974
H	0.742136	1.553369	0.481566
H	2.216511	-0.434250	0.552350
H	1.231912	-2.704842	0.585222
H	-1.226774	-2.988444	0.548637
H	-2.701122	-1.001350	0.479815
H	-1.716974	1.269401	0.445920
C	0.170468	0.506132	4.834694
C	1.616717	0.684919	4.379733
C	0.116077	0.474761	6.359559
C	-0.378912	-0.803360	4.274398

C	-0.670905	1.670704	4.318489
H	2.032573	1.618197	4.763156
H	2.240116	-0.135696	4.738586
H	1.677326	0.704311	3.290798
H	-0.909713	0.347340	6.708647
H	0.711483	-0.350926	6.752113
H	0.504371	1.402645	6.782465
H	-1.413786	-0.953635	4.587070
H	0.207545	-1.652334	4.630209
H	-0.350132	-0.803813	3.184084
H	-0.649364	1.706734	3.228490
H	-1.710694	1.566934	4.632971
H	-0.295252	2.621398	4.700595

107 U···pentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.208905	-0.964583	0.534761
C	-1.446342	-0.344581	0.306659
O	-2.461237	-1.010792	0.197892
C	-1.357782	1.103186	0.228144
C	-0.163003	1.709893	0.381126
N	0.985452	1.000824	0.611206
C	1.027021	-0.379170	0.712647
O	2.049197	-0.997395	0.937260
H	-0.224151	-1.973109	0.605084
H	-2.256572	1.667731	0.049847
H	-0.046290	2.782446	0.333350
H	1.867560	1.466928	0.744784
C	1.141412	2.357032	4.057078
C	1.214429	0.838161	4.146597
C	-0.150356	0.179994	3.991780
C	-0.094067	-1.340693	4.051415
C	-1.463350	-1.982566	3.867642
H	0.710564	2.668080	3.104296
H	0.507179	2.762465	4.845326
H	2.124292	2.817479	4.150200
H	1.644813	0.548598	5.107887
H	1.889019	0.447000	3.381478
H	-0.821601	0.548870	4.773399
H	-0.597827	0.490259	3.041880
H	0.329538	-1.643123	5.012051
H	0.597454	-1.702572	3.286913
H	-1.901729	-1.709108	2.907456
H	-1.406411	-3.069334	3.911699

H	-2.151313	-1.654220	4.646875

108 U···cyclopentane

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.195730	-0.844689	0.823846
C	-1.179049	-0.573684	0.759483
O	-1.993646	-1.456265	0.966901
C	-1.476715	0.811156	0.437560
C	-0.468113	1.682962	0.234891
N	0.845629	1.305991	0.326831
C	1.254261	0.019462	0.636244
O	2.422304	-0.301716	0.731879
H	0.450398	-1.796753	1.049768
H	-2.506356	1.115651	0.363895
H	-0.638435	2.721643	-0.006164
H	1.589693	1.968879	0.185960
C	1.056723	-0.863510	4.398744
C	1.111037	0.602442	4.831680
C	-0.056315	1.215256	4.060908
C	-1.173259	0.177684	4.231937
C	-0.450223	-1.188864	4.335594
H	1.510576	-0.955567	3.410761
H	1.601226	-1.527491	5.067941
H	2.069327	1.075341	4.620955
H	0.922921	0.684079	5.904903
H	0.217989	1.304038	3.007437
H	-0.340729	2.206397	4.412542
H	-1.898799	0.201298	3.420565
H	-1.717345	0.382381	5.154185
H	-0.692888	-1.833020	3.492234
H	-0.765329	-1.716266	5.234680

109 U···neopentane

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	0.626081	-0.850913	0.805916
C	-0.432456	-0.087336	0.294664
O	-1.530772	-0.588403	0.123593
C	-0.066875	1.291275	0.019637
C	1.183542	1.717935	0.290533
N	2.134130	0.886602	0.819082
C	1.902783	-0.443178	1.128312

O	2.743806	-1.163924	1.628587
H	0.409190	-1.811501	1.034401
H	-0.809744	1.951810	-0.392840
H	1.501850	2.733871	0.109833
H	3.055336	1.223901	1.043428
C	-0.623702	-0.029718	4.731889
C	-1.940448	0.711571	4.946762
C	-0.008266	-0.383156	6.083167
C	0.341422	0.863760	3.956100
C	-0.885019	-1.309752	3.941524
H	-2.647520	0.093365	5.501624
H	-1.780949	1.631755	5.510947
H	-2.398158	0.973068	3.991608
H	0.934897	-0.915529	5.952385
H	0.188755	0.516586	6.667969
H	-0.679560	-1.020893	6.659903
H	1.289993	0.351165	3.785746
H	0.546712	1.781896	4.509526
H	-0.080973	1.142246	2.988636
H	-1.348758	-1.087919	2.978900
H	0.047557	-1.848151	3.761888
H	-1.555527	-1.971566	4.491709

110 PHE···ethene

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.835517	1.115167	0.021401
C	1.383275	-0.166147	0.023765
C	0.547555	-1.281316	0.021686
C	-0.835523	-1.115162	0.021399
C	-1.383284	0.166154	0.023758
C	-0.547566	1.281323	0.021680
H	1.484324	1.980609	0.019534
H	2.457149	-0.295205	0.022771
H	0.972936	-2.275805	0.019779
H	-1.484334	-1.980606	0.019530
H	-2.457156	0.295209	0.022757
H	-0.972943	2.275805	0.019769
C	0.655781	-0.116790	3.530752
C	-0.655776	0.116792	3.530761
H	1.047241	-1.123909	3.526283
H	1.370854	0.693273	3.526250
H	-1.370848	-0.693272	3.526265
H	-1.047239	1.123911	3.526302

111 U···ethene

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.050874	-0.980081	0.033962
C	-1.308813	-0.361876	0.004026
O	-2.327220	-1.032555	-0.005829
C	-1.236818	1.088048	-0.012224
C	-0.035194	1.697836	0.033705
N	1.134529	0.990283	0.091845
C	1.193186	-0.391833	0.115775
O	2.236398	-1.011188	0.194186
H	-0.053222	-1.990694	0.049822
H	-2.152739	1.651460	-0.054774
H	0.070366	2.772476	0.031882
H	2.023720	1.456772	0.155693
C	0.726007	0.025053	3.398190
C	-0.602769	0.125644	3.348944
H	1.243125	-0.845934	3.020964
H	1.331618	0.812048	3.825505
H	-1.214772	-0.661836	2.932043
H	-1.114594	0.996714	3.732943

112 neopentane···neopentane

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.382522	-0.070607	0.766896
C	-1.040639	0.396811	1.060936
C	0.590847	-1.466818	1.347978
C	1.378269	0.898435	1.399149
C	0.601961	-0.111034	-0.743097
H	-1.771575	-0.281500	0.618330
H	-1.224718	0.435735	2.135519
H	-1.214066	1.393724	0.653091
H	1.602914	-1.822950	1.150103
H	0.438969	-1.466746	2.428287
H	-0.109919	-2.178684	0.909314
H	2.404394	0.585441	1.200734
H	1.243781	0.945974	2.480710
H	1.248373	1.905023	0.998951
H	0.459212	0.877039	-1.182898
H	1.613694	-0.443459	-0.979672
H	-0.099531	-0.797550	-1.219221
C	-0.375028	0.069314	5.966488
C	1.047784	-0.399652	5.673089

C	-0.581425	1.465875	5.385658
C	-0.595323	0.109490	7.476342
C	-1.371491	-0.898464	5.333342
H	1.232223	-0.438982	4.598568
H	1.779218	0.278020	6.115824
H	1.220048	-1.396658	6.081209
H	-1.593388	1.822861	5.582505
H	0.119493	2.176947	5.825380
H	-0.428316	1.466072	4.305516
H	-1.606539	0.443767	7.712415
H	0.107190	0.794439	7.953180
H	-0.454760	-0.879030	7.915794
H	-1.242565	-1.905439	5.732921
H	-2.397380	-0.584691	5.531730
H	-1.236787	-0.945438	4.251765

113 cyclopentane···neopentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.799914	-1.022052	0.687737
C	1.116887	0.424953	1.099662
C	-0.244559	1.165690	1.102977
C	-1.298714	0.103812	0.739309
C	-0.646880	-1.220068	1.136307
H	0.853556	-1.122051	-0.398014
H	1.491402	-1.744169	1.119720
H	1.838142	0.890145	0.430453
H	1.555570	0.439825	2.097084
H	-0.258078	2.000863	0.405323
H	-0.448804	1.576996	2.090984
H	-1.473561	0.105243	-0.338005
H	-2.256734	0.278041	1.227158
H	-1.124439	-2.087627	0.682993
H	-0.686019	-1.345283	2.220220
C	0.049846	0.094208	5.616277
C	-0.046498	-0.057878	7.131918
C	0.763899	1.401113	5.280652
C	-1.355166	0.114032	5.018958
C	0.837746	-1.079277	5.038939
H	0.946048	-0.073345	7.584275
H	-0.605423	0.770006	7.570353
H	-0.553663	-0.986544	7.397267
H	0.845419	1.534612	4.200971
H	0.220427	2.255801	5.686154
H	1.771504	1.411763	5.698885

H	-1.318234	0.231222	3.935109
H	-1.937465	0.941456	5.427304
H	-1.885069	-0.813755	5.240287
H	0.342526	-2.026268	5.259182
H	0.932589	-0.992095	3.955804
H	1.842464	-1.116682	5.462688

114 cyclopentane···cyclopentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.956880	-0.891846	1.141950
C	0.990949	0.658508	1.145504
C	-0.479452	1.102319	1.103879
C	-1.182107	-0.052797	0.393346
C	-0.530660	-1.274890	1.039310
H	1.504566	-1.278358	0.283420
H	1.421384	-1.314778	2.031025
H	1.510594	1.023096	0.259948
H	1.516258	1.059818	2.010537
H	-0.616269	2.064877	0.613567
H	-0.874742	1.189071	2.118070
H	-0.948882	-0.026830	-0.673805
H	-2.265665	-0.033565	0.501274
H	-0.690391	-2.197021	0.482992
H	-0.950849	-1.415412	2.036748
C	-1.131985	-0.383919	5.055966
C	0.181621	-1.179463	5.008205
C	1.310937	-0.116758	5.008801
C	0.600763	1.244911	5.116668
C	-0.741289	0.910439	5.766480
H	-1.465120	-0.147220	4.043382
H	-1.936774	-0.927017	5.548953
H	0.231566	-1.837206	4.142071
H	0.261909	-1.810821	5.892590
H	1.932201	-0.177436	4.116928
H	1.968346	-0.266641	5.864206
H	0.420900	1.653403	4.120669
H	1.181147	1.979315	5.672641
H	-1.480958	1.702950	5.661599
H	-0.601249	0.718799	6.833029

115 pentane···pentane

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
C	-2.533309	-0.294879	0.713149
C	-1.271885	0.557655	0.674355
C	-0.000135	-0.278418	0.719603
C	1.271895	0.557382	0.674061
C	2.533404	-0.294942	0.713280
H	-2.563627	-0.977082	-0.136423
H	-2.566978	-0.895876	1.621732
H	-3.434426	0.315957	0.684104
H	-1.271026	1.256566	1.514319
H	-1.266633	1.167896	-0.231827
H	-0.000159	-0.887230	1.628637
H	-0.000365	-0.980714	-0.119404
H	1.270972	1.256633	1.513705
H	1.266636	1.167183	-0.232387
H	2.563919	-0.977774	-0.135778
H	3.434310	0.316254	0.683599
H	2.567558	-0.895209	1.622329
C	2.533557	0.295021	4.513100
C	1.271731	-0.556866	4.552404
C	-0.000044	0.279233	4.506788
C	-1.271805	-0.556909	4.552059
C	-2.533524	0.295137	4.513082
H	2.568142	0.894828	3.603774
H	2.564061	0.978228	5.361845
H	3.434238	-0.316476	4.543309
H	1.266287	-1.166594	5.458901
H	1.270601	-1.256220	3.712823
H	-0.000199	0.981543	5.345772
H	0.000033	0.888010	3.597718
H	-1.266422	-1.167018	5.458309
H	-1.270698	-1.255932	3.712196
H	-2.567717	0.895671	3.604205
H	-3.434326	-0.316161	4.542595
H	-2.564063	0.977724	5.362343

116 peptide···pentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	1.372191	1.012477	0.970825
C	0.326737	-0.077647	0.988199
O	0.618821	-1.252481	1.171281
N	-0.950029	0.344887	0.773915
C	-2.059854	-0.577369	0.680153
H	0.952176	2.014050	1.033117

H	1.947422	0.926516	0.050718
H	2.051702	0.851825	1.802952
H	-1.104672	1.322025	0.606112
H	-1.669356	-1.566796	0.897184
H	-2.834592	-0.331380	1.403661
H	-2.490971	-0.578925	-0.319939
C	2.660666	0.462745	4.853346
C	1.432393	-0.400642	4.595795
C	0.149855	0.417972	4.530494
C	-1.094501	-0.432363	4.313614
C	-2.361339	0.407928	4.223499
H	2.777505	1.217161	4.074602
H	2.574555	0.987632	5.805003
H	3.572757	-0.131497	4.880154
H	1.337824	-1.146096	5.388846
H	1.548813	-0.954106	3.661951
H	0.038285	0.995707	5.453577
H	0.229090	1.150787	3.720841
H	-1.185303	-1.146850	5.135031
H	-0.966694	-1.021301	3.403399
H	-2.294426	1.114979	3.395730
H	-3.246682	-0.208089	4.069666
H	-2.511695	0.984139	5.136719

117 pentane···AcOH

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.275345	-0.135075	0.831334
C	-0.961698	0.619278	0.669399
C	0.226502	-0.314710	0.479986
C	1.543002	0.421175	0.269000
C	2.727576	-0.526861	0.137459
H	-2.490718	-0.727927	-0.057566
H	-2.226324	-0.818446	1.678823
H	-3.112026	0.544943	0.987400
H	-0.788699	1.250432	1.544703
H	-1.026177	1.295445	-0.186458
H	0.309444	-0.975139	1.348038
H	0.039151	-0.965999	-0.378790
H	1.711639	1.107772	1.102447
H	1.466095	1.043743	-0.625294
H	2.588742	-1.203214	-0.705757
H	3.661501	0.011693	-0.015969
H	2.835194	-1.137410	1.034075
C	-0.483561	-0.287863	4.121252

O	-0.906175	-1.403043	3.924105
O	-1.297254	0.771102	4.353841
C	0.956706	0.121803	4.138457
H	-2.198016	0.416722	4.313305
H	1.582529	-0.748378	3.980302
H	1.132743	0.856077	3.355332
H	1.194017	0.591104	5.090259

118 pentane···$AcNH_2$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.587776	-0.323106	0.469458
C	-1.309560	0.497394	0.585063
C	-0.056830	-0.368260	0.558440
C	1.231596	0.440066	0.632032
C	2.472575	-0.443144	0.619221
H	-2.610389	-0.876366	-0.469619
H	-2.659744	-1.051887	1.277714
H	-3.476035	0.305625	0.508961
H	-1.317251	1.083262	1.506341
H	-1.262377	1.215574	-0.236776
H	-0.086175	-1.073359	1.395875
H	-0.053809	-0.976843	-0.351474
H	1.213283	1.053562	1.534593
H	1.266297	1.131377	-0.213106
H	2.520719	-1.035263	-0.294897
H	3.387734	0.144090	0.683909
H	2.459297	-1.139364	1.458618
C	0.042162	0.201242	4.116508
O	0.069074	1.386316	3.824667
N	1.174742	-0.550636	4.219328
C	-1.248059	-0.537695	4.380962
H	2.045683	-0.128055	3.950666
H	1.135805	-1.542522	4.350751
H	-1.100809	-1.498417	4.868086
H	-1.754286	-0.696004	3.430149
H	-1.886003	0.089541	4.996234

119 ethene···pentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.666400	0.183811	0.419737
C	-0.665974	0.182973	0.419612

H	1.228882	-0.329883	1.186260
H	1.228036	0.697208	-0.347610
H	-1.227922	-0.331499	1.186103
H	-1.228184	0.695646	-0.347748
C	-2.532760	-0.393659	4.145342
C	-1.271323	0.459016	4.181160
C	-0.000049	-0.378541	4.154217
C	1.271171	0.459045	4.181622
C	2.532623	-0.393679	4.145798
H	-2.562253	-1.006680	3.244153
H	-2.568894	-1.067880	5.000959
H	-3.433931	0.217357	4.162588
H	-1.271729	1.079110	5.080554
H	-1.262935	1.145925	3.332100
H	-0.000203	-1.065214	5.006049
H	0.000092	-1.006119	3.257575
H	1.271444	1.078856	5.081107
H	1.262976	1.146120	3.332714
H	2.562246	-1.006536	3.244488
H	3.433801	0.217257	4.163376
H	2.568541	-1.068136	5.001303

120 ethyne···pentane

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.606189	0.055874	0.589005
C	0.605849	0.055541	0.589266
H	-1.668037	0.055776	0.589012
H	1.667678	0.054863	0.589728
C	-2.530404	-0.347456	4.218514
C	-1.269872	0.507145	4.229583
C	0.000047	-0.331186	4.270039
C	1.269945	0.507190	4.229670
C	2.530468	-0.347447	4.218724
H	-2.538771	-1.009410	3.352104
H	-2.582322	-0.973725	5.109105
H	-3.432819	0.261448	4.185753
H	-1.286523	1.180144	5.089993
H	-1.244605	1.141361	3.340787
H	0.000050	-0.948976	5.173100
H	0.000114	-1.019485	3.420798
H	1.286573	1.180157	5.090092
H	1.244800	1.141362	3.340869
H	2.538848	-1.009430	3.352345
H	3.432847	0.261485	4.185998

H	2.582285	-0.973662	5.109357

121 pyrene···methane

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.651669	0.000029	-0.342241
C	1.377620	1.256558	-0.368431
C	2.803320	1.231938	-0.421591
C	3.505939	0.000047	-0.447071
C	1.377629	-1.256492	-0.368511
C	2.803339	-1.231862	-0.421661
C	0.626651	2.501269	-0.327521
C	0.626678	-2.501211	-0.327661
C	-0.788761	0.000019	-0.270151
C	-1.514281	-1.256660	-0.227351
C	-2.939031	-1.231840	-0.150321
C	-3.641031	0.000000	-0.113101
C	-1.514300	1.256690	-0.227281
C	-2.939040	1.231840	-0.150251
C	-0.762522	-2.501441	-0.259331
C	-0.762539	2.501479	-0.259191
H	3.353190	2.186558	-0.439551
H	4.605449	0.000047	-0.486271
H	3.353208	-2.186472	-0.439681
H	1.184181	3.451709	-0.348401
H	1.184218	-3.451651	-0.348591
H	-3.488292	-2.186409	-0.118321
H	-4.739571	-0.000009	-0.053331
H	-3.488310	2.186411	-0.118201
H	-1.319312	-3.451990	-0.226751
H	-1.319349	3.452020	-0.226561
C	0.720789	-0.000241	3.090639
H	0.760799	-0.000361	4.194139
H	1.745859	-0.000022	2.681179
H	0.187719	-0.900231	2.738149
H	0.187430	0.899659	2.738359

122 pyridine···pyridine

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	-0.941211	0.790041	0.011719
C	-0.922755	-0.552378	0.035379
C	-2.076519	-1.333018	0.039290

C	-3.316313	-0.703340	0.017599
C	-3.348895	0.687019	-0.007086
C	-2.143104	1.382634	-0.008890
H	0.057241	-1.015588	0.051355
H	-1.996529	-2.410586	0.058877
H	-4.231575	-1.279084	0.019794
H	-4.285444	1.226105	-0.024659
H	-2.138100	2.465653	-0.027783
N	2.533211	-0.950029	0.042518
C	3.734990	-1.543206	0.044598
C	4.940926	-0.848247	0.020596
C	4.908609	0.542057	-0.007150
C	3.668928	1.172344	-0.009627
C	2.515015	0.392334	0.015566
H	3.729766	-2.626168	0.066487
H	5.877365	-1.387782	0.023690
H	5.823984	1.117309	-0.026332
H	3.589156	2.249902	-0.030716
H	1.535104	0.855997	0.013903

123 ethyne···water

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.006867	-0.030568	-0.024773
C	-2.218744	0.003173	0.002599
H	0.059003	-0.060940	-0.049366
H	-3.279277	0.033525	0.027200
O	2.263905	-0.145570	-0.115471
H	2.834261	-0.735339	0.381556
H	2.835900	0.205418	-0.800843

124 pyridine···ethyne

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-0.083032	0.000715	1.055200
C	-0.202854	-1.141726	0.364934
C	-0.446781	-1.191764	-1.004512
C	-0.574682	0.003440	-1.704309
C	-0.453457	1.197243	-1.000916
C	-0.209311	1.144508	0.368367
H	-0.098486	-2.055098	0.937433
H	-0.533649	-2.145855	-1.504172
H	-0.763684	0.004480	-2.768727

H	-0.545631	2.152273	-1.497795
H	-0.110167	2.056697	0.943574
C	0.471836	-0.006058	5.541719
C	0.339766	-0.006608	4.335472
H	0.587246	-0.005484	6.596733
H	0.221618	-0.006345	3.270966

Table S25. Cartesian x, y, z coordinates in angstroms for the 14 large noncovalent complexes.

125 antiparallel Gly pentapeptide dimer

Atomic Number	Coordinates (Angstroms) X	Y	Z
N	8.320866	1.425969	0.000000
C	9.762237	1.260197	0.000000
C	7.480240	0.370792	0.000000
O	7.825034	-0.820781	0.000000
C	6.006032	0.759069	0.000000
N	5.220426	-0.453274	0.000000
C	3.879977	-0.405690	0.000000
O	3.251788	0.669045	0.000000
C	3.163221	-1.748478	0.000000
N	1.740199	-1.510326	0.000000
C	0.871916	-2.539763	0.000000
O	1.216622	-3.731440	0.000000
C	-0.596635	-2.132795	0.000000
N	-1.395229	-3.334935	0.000000
C	-2.738730	-3.291629	0.000000
O	-3.372075	-2.219284	0.000000
C	-3.424549	-4.645706	0.000000
N	-4.855324	-4.480809	0.000000
C	-5.639632	-5.592095	0.000000
O	-5.153888	-6.729555	0.000000
C	-7.132372	-5.347193	0.000000
H	7.916767	2.361916	0.000000
H	10.204612	1.715528	0.890392
H	10.204612	1.715528	-0.890392
H	9.971630	0.191017	0.000000
H	5.779366	1.374696	0.875817
H	5.779366	1.374696	-0.875817
H	5.756553	-1.319056	0.000000
H	3.461176	-2.333770	0.879437
H	3.461176	-2.333770	-0.879437
H	1.418036	-0.541883	0.000000
H	-0.812366	-1.513514	0.876171
H	-0.812366	-1.513514	-0.876171
H	-0.869442	-4.206677	0.000000
H	-3.102451	-5.223758	-0.876369
H	-3.102451	-5.223758	0.876369
H	-5.237290	-3.538476	0.000000
H	-7.563475	-5.828589	0.881301
H	-7.563475	-5.828589	-0.881301
H	-7.375677	-4.284707	0.000000
O	6.610842	3.822209	0.000000
C	5.981006	4.896697	0.000000

C	6.690918	6.230328	0.000000
N	4.635476	4.930654	0.000000
C	3.847951	3.721163	0.000000
C	2.376284	4.114567	0.000000
O	2.019884	5.303490	0.000000
N	1.514998	3.079162	0.000000
C	0.091412	3.313911	0.000000
C	-0.625466	1.971649	0.000000
O	0.000000	0.896854	0.000000
N	-1.967305	2.021427	0.000000
C	-2.756334	0.810361	0.000000
C	-4.224215	1.207371	0.000000
O	-4.574130	2.398809	0.000000
N	-5.098132	0.181909	0.000000
C	-6.510427	0.467091	0.000000
C	-7.300532	-0.833421	0.000000
O	-6.748896	-1.940518	0.000000
N	-8.644769	-0.656081	0.000000
C	-9.595333	-1.754920	0.000000
H	7.332865	6.286599	0.882133
H	6.003741	7.078951	0.000000
H	7.332865	6.286599	-0.882133
H	4.101425	5.795419	0.000000
H	4.071056	3.103294	0.875409
H	4.071056	3.103294	-0.875409
H	1.843746	2.112349	0.000000
H	-0.207266	3.899180	0.879304
H	-0.207266	3.899180	-0.879304
H	-2.497840	2.890025	0.000000
H	-2.534276	0.192570	0.875372
H	-2.534276	0.192570	-0.875372
H	-4.787694	-0.791821	0.000000
H	-6.781372	1.067123	-0.878840
H	-6.781372	1.067123	0.878840
H	-9.002333	0.290948	0.000000
H	-10.226471	-1.720013	-0.891716
H	-10.226471	-1.720013	0.891716
H	-9.026132	-2.682233	0.000000

126 parallel Gly pentapeptide dimer

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
N	-8.313542	-1.706309	0.000000
C	-6.959908	-1.715946	0.000000
O	-6.275204	-2.749726	0.000000

C	-6.339538	-0.327406	0.000000
N	-4.899038	-0.396032	0.000000
C	-4.197730	0.763293	0.000000
O	-4.747238	1.874078	0.000000
C	-2.690464	0.607316	0.000000
N	-2.084781	1.916824	0.000000
C	-0.743273	2.025517	0.000000
O	0.000000	1.028658	0.000000
C	-0.195587	3.442534	0.000000
N	1.246370	3.410503	0.000000
C	1.939851	4.571558	0.000000
O	1.389483	5.683071	0.000000
C	3.446526	4.410205	0.000000
N	4.058502	5.714438	0.000000
C	5.404568	5.814192	0.000000
O	6.129218	4.804771	0.000000
C	-9.125711	-2.911097	0.000000
C	5.982292	7.210912	0.000000
H	-8.785126	-0.810110	0.000000
H	-6.692226	0.230325	0.877722
H	-6.692226	0.230325	-0.877722
H	-4.431440	-1.300428	0.000000
H	-2.369791	0.028997	0.871314
H	-2.369791	0.028997	-0.871314
H	-2.716422	2.713066	0.000000
H	-0.569517	3.985019	0.878217
H	-0.569517	3.985019	-0.878217
H	1.722194	2.509407	0.000000
H	3.766699	3.828476	-0.869505
H	3.766699	3.828476	0.869505
H	3.431530	6.511992	0.000000
H	-9.755742	-2.952002	-0.891855
H	-9.755742	-2.952002	0.891855
H	-8.450688	-3.764709	0.000000
H	6.616007	7.329034	0.881867
H	5.215350	7.988787	0.000000
H	6.616007	7.329034	-0.881867
N	-5.692660	-5.779277	0.000000
C	-4.339123	-5.775618	0.000000
O	-3.621201	-6.783382	0.000000
C	-3.748281	-4.375250	0.000000
N	-2.309804	-4.466138	0.000000
C	-1.588896	-3.332517	0.000000
O	-2.134941	-2.213570	0.000000
C	-0.078428	-3.488928	0.000000
N	0.539574	-2.184786	0.000000

C	1.887594	-2.080750	0.000000
O	2.640554	-3.065000	0.000000
C	2.414817	-0.657193	0.000000
N	3.855564	-0.694087	0.000000
C	4.556645	0.457449	0.000000
O	3.993964	1.566236	0.000000
C	6.063831	0.293006	0.000000
N	6.739688	1.567011	0.000000
C	8.102545	1.555709	0.000000
O	8.731532	0.488883	0.000000
C	-6.464539	-7.007488	0.000000
C	8.794107	2.899463	0.000000
H	-6.160611	-4.876454	0.000000
H	-4.100365	-3.819750	0.875344
H	-4.100365	-3.819750	-0.875344
H	-1.912422	-5.402331	0.000000
H	0.236748	-4.066975	0.878442
H	0.236748	-4.066975	-0.878442
H	-0.057589	-1.358979	0.000000
H	2.035989	-0.116121	-0.872840
H	2.035989	-0.116121	0.872840
H	4.286010	-1.614774	0.000000
H	6.366349	-0.298556	0.874593
H	6.366349	-0.298556	-0.874593
H	6.199929	2.430115	0.000000
H	-7.094761	-7.073349	-0.891483
H	-7.094761	-7.073349	0.891483
H	-5.757080	-7.836234	0.000000
H	9.440457	2.949867	0.880079
H	8.100444	3.739780	0.000000
H	9.440457	2.949867	-0.880079

127 parallel Ala tripeptide dimer

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-5.022037	1.924695	-1.396792
C	-3.889160	2.645375	-0.696434
O	-3.800720	3.878677	-0.679601
N	-2.965890	1.822064	-0.119738
C	-1.828165	2.350166	0.596035
C	-0.553075	1.805982	-0.029158
O	-0.463782	0.598831	-0.325109
C	-1.871628	1.968691	2.077051
N	0.444916	2.690773	-0.218705
C	1.773724	2.299702	-0.661703

C	2.760641	2.796533	0.388295
O	2.662331	3.947186	0.837884
C	2.101387	2.916679	-2.019298
N	3.720592	1.906497	0.732221
C	4.752639	2.230806	1.698603
H	-5.070064	0.866696	-1.131862
H	-5.959526	2.420865	-1.138164
H	-4.883244	2.020724	-2.477499
H	-3.105895	0.812261	-0.122352
H	-1.879620	3.437621	0.481590
H	-0.993243	2.351187	2.607650
H	-2.772072	2.386665	2.533909
H	-1.897753	0.880282	2.178110
H	0.352192	3.643120	0.123486
H	1.782154	1.210142	-0.723423
H	1.366498	2.596625	-2.762291
H	3.098115	2.604335	-2.345972
H	2.084323	4.007433	-1.944091
H	3.658225	0.961060	0.360899
H	4.645590	1.627188	2.605212
H	5.746154	2.062694	1.273493
H	4.641261	3.283850	1.955789
C	-4.850966	-3.201084	-0.100077
C	-3.709935	-2.269290	0.242363
O	-3.806701	-1.046809	0.053264
N	-2.613516	-2.855216	0.787552
C	-1.377965	-2.131015	1.030792
C	-0.270012	-2.862777	0.284696
O	-0.185547	-4.100483	0.341213
C	-1.046977	-2.071872	2.520457
N	0.587618	-2.065671	-0.395519
C	1.716815	-2.614838	-1.115443
C	2.994523	-1.973075	-0.597013
O	3.086654	-0.741844	-0.462950
C	1.592457	-2.352034	-2.617012
N	4.036344	-2.804919	-0.376819
C	5.317870	-2.296564	0.085453
H	-5.746344	-2.861791	0.425244
H	-5.049145	-3.131153	-1.172277
H	-4.650719	-4.241954	0.163391
H	-2.528330	-3.866836	0.785269
H	-1.507552	-1.125982	0.626158
H	-0.126582	-1.501423	2.681577
H	-0.907387	-3.083290	2.912822
H	-1.862541	-1.587472	3.063721
H	0.422685	-1.055792	-0.424465

H	1.708262	-3.691085	-0.915192
H	2.452650	-2.760045	-3.157353
H	1.542126	-1.274934	-2.797711
H	0.680149	-2.819389	-2.994936
H	3.871389	-3.802831	-0.383883
H	5.257698	-1.944551	1.119545
H	6.056266	-3.095626	0.017589
H	5.625111	-1.464227	-0.549444

128 anthracene dimer st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.856445	-1.338599	-2.177360
C	1.533794	-0.996582	-0.732914
C	-0.329315	-2.422415	-1.463206
C	1.008847	0.086170	-1.448804
C	-0.220485	-0.090363	-2.194436
C	0.904424	-2.247566	-0.724268
C	-0.968284	-3.699203	-1.434777
C	1.640938	1.365785	-1.463800
C	-0.744111	1.021622	-2.921468
C	1.434440	-3.359666	-0.004419
C	-0.425887	-4.743926	-0.726933
C	1.106788	2.408723	-2.177516
C	-0.099542	2.233836	-2.914988
C	0.792023	-4.573238	-0.005818
H	-1.782630	-1.470087	-2.734365
H	2.450523	-0.860964	-0.163415
H	-1.896039	-3.827980	-1.988222
H	2.551735	1.500161	-0.886136
H	-1.667812	0.887909	-3.480648
H	2.356472	-3.221609	0.554765
H	-0.922956	-5.710773	-0.715905
H	1.590367	3.381001	-2.165326
H	-0.513616	3.073700	-3.466686
H	1.207049	-5.410914	0.548928
C	-1.533794	0.996582	0.732914
C	0.856445	1.338599	2.177360
C	-1.008847	-0.086170	1.448804
C	0.329315	2.422415	1.463206
C	-0.904424	2.247566	0.724268
C	0.220485	0.090363	2.194436
C	-1.640938	-1.365785	1.463800
C	0.968284	3.699203	1.434777
C	-1.434440	3.359666	0.004419

C	0.744111	-1.021622	2.921468
C	-1.106788	-2.408723	2.177516
C	0.425887	4.743926	0.726933
C	-0.792023	4.573238	0.005818
C	0.099542	-2.233836	2.914988
H	-2.450523	0.860964	0.163415
H	1.782630	1.470087	2.734365
H	-2.551735	-1.500161	0.886136
H	1.896039	3.827980	1.988222
H	-2.356472	3.221609	-0.554765
H	1.667812	-0.887909	3.480648
H	-1.590367	-3.381001	2.165326
H	0.922956	5.710773	0.715905
H	-1.207049	5.410914	-0.548928
H	0.513616	-3.073700	3.466686

129 tetracene dimer st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.897627	2.688409	-0.133191
C	2.693444	2.878884	-0.758987
C	1.486508	2.339852	-0.210195
C	1.565562	1.585766	1.030767
C	2.845948	1.409548	1.643518
C	3.975753	1.943745	1.083541
C	0.247611	2.513185	-0.825751
C	-0.935435	1.981716	-0.274756
C	-0.856455	1.229357	0.969656
C	0.401121	1.051607	1.579167
C	-2.192453	2.152808	-0.888721
C	-3.358219	1.628352	-0.332710
C	-3.279695	0.882577	0.913422
C	-2.039019	0.699141	1.521514
C	-4.485926	0.354000	1.470673
C	-5.693125	0.542269	0.849334
C	-5.769893	1.270047	-0.378676
C	-4.639049	1.795081	-0.948912
H	4.807425	3.096682	-0.565332
H	2.633418	3.442801	-1.687474
H	2.903687	0.827843	2.559892
H	4.942933	1.785299	1.551130
H	0.189308	3.076411	-1.755497
H	0.463246	0.475668	2.499726
H	-2.252021	2.711306	-1.821227
H	-1.978752	0.125294	2.443552

H	-4.421342	-0.210695	2.397398
H	-6.600998	0.133023	1.285033
H	-6.735986	1.407529	-0.858055
H	-4.696048	2.350802	-1.882430
C	-3.975753	-1.943745	-1.083541
C	-2.845948	-1.409548	-1.643518
C	-1.565562	-1.585766	-1.030767
C	-1.486508	-2.339852	0.210195
C	-2.693444	-2.878884	0.758987
C	-3.897627	-2.688409	0.133191
C	-0.247611	-2.513185	0.825751
C	0.935435	-1.981716	0.274756
C	0.856455	-1.229357	-0.969656
C	-0.401121	-1.051607	-1.579167
C	2.039019	-0.699141	-1.521514
C	3.279695	-0.882577	-0.913422
C	3.358219	-1.628352	0.332710
C	2.192453	-2.152808	0.888721
C	4.485926	-0.354000	-1.470673
C	5.693125	-0.542269	-0.849334
C	5.769893	-1.270047	0.378676
C	4.639049	-1.795081	0.948912
H	-4.942933	-1.785299	-1.551130
H	-2.903687	-0.827843	-2.559892
H	-2.633418	-3.442801	1.687474
H	-4.807425	-3.096682	0.565332
H	-0.189308	-3.076411	1.755497
H	-0.463246	-0.475668	-2.499726
H	1.978752	-0.125294	-2.443552
H	2.252021	-2.711306	1.821227
H	4.421342	0.210695	-2.397398
H	6.600998	-0.133023	-1.285033
H	6.735986	-1.407529	0.858055
H	4.696048	-2.350802	1.882430

130 coronene dimer st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.487532	-1.231543	-1.729000
C	-0.065468	-1.231543	-1.729000
C	0.645564	0.000000	-1.729000
C	-0.065468	1.231543	-1.729000
C	-1.487532	1.231543	-1.729000
C	-2.198564	0.000000	-1.729000
C	0.642292	-2.457420	-1.729000

C	-0.093378	-3.670823	-1.729000
C	-1.459622	-3.670823	-1.729000
C	-2.195292	-2.457420	-1.729000
C	-3.614084	0.000000	-1.729000
C	-4.297087	-1.243810	-1.729000
C	-3.613965	-2.427013	-1.729000
C	-4.297087	1.243810	-1.729000
C	-3.613965	2.427013	-1.729000
C	-2.195292	2.457420	-1.729000
C	-1.459622	3.670823	-1.729000
C	-0.093378	3.670823	-1.729000
C	0.642292	2.457420	-1.729000
C	2.060965	2.427013	-1.729000
C	2.744087	1.243810	-1.729000
C	2.061084	0.000000	-1.729000
C	2.744087	-1.243810	-1.729000
C	2.060965	-2.427013	-1.729000
H	0.449580	-4.607417	-1.729000
H	-2.002581	-4.607417	-1.729000
H	-5.379680	-1.241892	-1.729000
H	-4.153600	-3.365525	-1.729000
H	-5.379680	1.241892	-1.729000
H	-4.153600	3.365525	-1.729000
H	-2.002581	4.607417	-1.729000
H	0.449580	4.607417	-1.729000
H	2.600600	3.365525	-1.729000
H	3.826680	1.241892	-1.729000
H	3.826680	-1.241892	-1.729000
H	2.600600	-3.365525	-1.729000
C	0.065468	-1.231543	1.729000
C	1.487532	-1.231543	1.729000
C	2.198564	0.000000	1.729000
C	1.487532	1.231543	1.729000
C	0.065468	1.231543	1.729000
C	-0.645564	0.000000	1.729000
C	2.195292	-2.457420	1.729000
C	1.459622	-3.670823	1.729000
C	0.093378	-3.670823	1.729000
C	-0.642292	-2.457420	1.729000
C	-2.061084	0.000000	1.729000
C	-2.744087	-1.243810	1.729000
C	-2.060965	-2.427013	1.729000
C	-2.744087	1.243810	1.729000
C	-2.060965	2.427013	1.729000
C	-0.642292	2.457420	1.729000
C	0.093378	3.670823	1.729000

C	1.459622	3.670823	1.729000
C	2.195292	2.457420	1.729000
C	3.613965	2.427013	1.729000
C	4.297087	1.243810	1.729000
C	3.614084	0.000000	1.729000
C	4.297087	-1.243810	1.729000
C	3.613965	-2.427013	1.729000
H	2.002581	-4.607417	1.729000
H	-0.449580	-4.607417	1.729000
H	-3.826680	-1.241892	1.729000
H	-2.600600	-3.365525	1.729000
H	-3.826680	1.241892	1.729000
H	-2.600600	3.365525	1.729000
H	-0.449580	4.607417	1.729000
H	2.002581	4.607417	1.729000
H	4.153600	3.365525	1.729000
H	5.379680	1.241892	1.729000
H	5.379680	-1.241892	1.729000
H	4.153600	-3.365525	1.729000

131 adeninre···cicumcoronene st

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.230000	-0.152000	2.591000
C	-0.950000	-0.739000	2.643000
C	0.131000	0.153000	2.667000
C	-1.196000	1.917000	2.639000
C	0.791000	-1.962000	2.624000
N	-2.328000	1.192000	2.594000
N	0.075000	1.492000	2.674000
N	-0.520000	-2.058000	2.616000
N	1.248000	-0.659000	2.668000
N	-3.378000	-0.885000	2.563000
H	-1.335000	2.995000	2.632000
H	1.478000	-2.796000	2.584000
H	2.209000	-0.350000	2.597000
H	-4.215000	-0.388000	2.285000
H	-3.310000	-1.855000	2.283000
C	6.220000	-1.272000	-0.103000
C	6.356000	0.086000	-0.067000
C	5.220000	0.956000	-0.165000
C	3.923000	0.366000	-0.304000
C	3.782000	-1.049000	-0.351000
C	4.934000	-1.892000	-0.240000
C	2.493000	-1.631000	-0.480000

C	4.770000	-3.283000	-0.265000
C	3.506000	-3.877000	-0.385000
C	2.348000	-3.043000	-0.500000
C	3.325000	-5.299000	-0.390000
C	2.082000	-5.857000	-0.476000
C	0.902000	-5.047000	-0.564000
C	1.053000	-3.625000	-0.579000
C	-0.094000	-2.794000	-0.668000
C	0.051000	-1.376000	-0.669000
C	1.342000	-0.795000	-0.596000
C	2.777000	1.198000	-0.411000
C	1.483000	0.616000	-0.539000
C	0.335000	1.447000	-0.612000
C	-0.954000	0.866000	-0.706000
C	-1.098000	-0.545000	-0.714000
C	-1.388000	-3.374000	-0.698000
C	-2.540000	-2.541000	-0.725000
C	-2.397000	-1.129000	-0.764000
C	-0.384000	-5.600000	-0.613000
C	-1.531000	-4.796000	-0.667000
C	-3.848000	-3.122000	-0.735000
C	-4.970000	-2.283000	-0.758000
C	-4.850000	-0.887000	-0.776000
C	-3.547000	-0.297000	-0.768000
C	-2.110000	1.699000	-0.715000
C	-3.403000	1.117000	-0.763000
C	-2.853000	-5.350000	-0.684000
C	-3.959000	-4.551000	-0.713000
C	-4.561000	1.957000	-0.756000
C	-5.853000	1.338000	-0.775000
C	-5.992000	-0.020000	-0.782000
C	-4.398000	3.348000	-0.723000
C	-3.131000	3.942000	-0.678000
C	-1.967000	3.110000	-0.676000
C	-0.674000	3.692000	-0.579000
C	0.478000	2.863000	-0.555000
C	1.768000	3.443000	-0.435000
C	2.916000	2.610000	-0.345000
C	4.218000	3.190000	-0.215000
C	5.337000	2.351000	-0.126000
C	4.325000	4.619000	-0.169000
C	1.904000	4.865000	-0.368000
C	3.221000	5.418000	-0.243000
C	-0.527000	5.114000	-0.521000
C	0.756000	5.667000	-0.421000
C	-2.953000	5.364000	-0.625000

C	-1.710000	5.923000	-0.552000
H	7.095000	-1.912000	-0.024000
H	7.340000	0.535000	0.037000
H	5.648000	-3.920000	-0.181000
H	4.205000	-5.932000	-0.315000
H	1.965000	-6.939000	-0.470000
H	-0.497000	-6.682000	-0.594000
H	-5.963000	-2.729000	-0.763000
H	-2.959000	-6.432000	-0.666000
H	-4.953000	-4.992000	-0.720000
H	-6.732000	1.979000	-0.778000
H	-6.982000	-0.470000	-0.790000
H	-5.281000	3.984000	-0.719000
H	6.324000	2.797000	-0.023000
H	5.314000	5.059000	-0.070000
H	3.324000	6.500000	-0.201000
H	0.865000	6.749000	-0.375000
H	-3.838000	5.995000	-0.639000
H	-1.596000	7.004000	-0.509000

132 anthracene dimer TS

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.477032	1.409326	-2.468552
C	-3.660752	0.712890	-2.462070
C	-3.660752	-0.712890	-2.462070
C	-2.477032	-1.409326	-2.468552
C	-1.223444	-0.724772	-2.479047
C	-1.223444	0.724772	-2.479047
C	0.000000	-1.408007	-2.476769
C	0.000000	1.408007	-2.476769
C	1.223444	0.724772	-2.479047
C	1.223444	-0.724772	-2.479047
C	2.477032	1.409326	-2.468552
C	2.477032	-1.409326	-2.468552
C	3.660752	0.712890	-2.462070
C	3.660752	-0.712890	-2.462070
H	-2.474378	2.496651	-2.459414
H	-4.606752	1.247487	-2.449607
H	-4.606752	-1.247487	-2.449607
H	-2.474378	-2.496651	-2.459414
H	0.000000	-2.496024	-2.466885
H	0.000000	2.496024	-2.466885
H	2.474378	2.496651	-2.459414
H	2.474378	-2.496651	-2.459414

H	4.606752	1.247487	-2.449607
H	4.606752	-1.247487	-2.449607
C	-2.474607	0.000000	1.054777
C	-3.659182	0.000000	1.749609
C	-3.662086	0.000000	3.175976
C	-2.479317	0.000000	3.875009
C	-1.223813	0.000000	3.192799
C	-1.222870	0.000000	1.742861
C	0.000000	0.000000	3.876507
C	0.000000	0.000000	1.058175
C	1.222870	0.000000	1.742861
C	1.223813	0.000000	3.192799
C	2.474607	0.000000	1.054777
C	2.479317	0.000000	3.875009
C	3.659182	0.000000	1.749609
C	3.662086	0.000000	3.175976
H	-2.472082	0.000000	-0.030018
H	-4.603808	0.000000	1.211314
H	-4.609385	0.000000	3.709590
H	-2.479065	0.000000	4.962944
H	0.000000	0.000000	4.965252
H	0.000000	0.000000	-0.027593
H	2.472082	0.000000	-0.030018
H	2.479065	0.000000	4.962944
H	4.603808	0.000000	1.211314
H	4.609385	0.000000	3.709590

133 tetracene dimer TS

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-4.888505	-0.714879	2.461189
C	-3.707690	-1.411364	2.464642
C	-2.449998	-0.727671	2.472705
C	-2.449998	0.727671	2.472705
C	-3.707690	1.411364	2.464642
C	-4.888505	0.714879	2.461189
C	-1.233839	-1.410569	2.469793
C	0.000000	-0.728638	2.474386
C	0.000000	0.728638	2.474386
C	-1.233839	1.410569	2.469793
C	1.233839	-1.410569	2.469793
C	2.449998	-0.727671	2.472705
C	2.449998	0.727671	2.472705
C	1.233839	1.410569	2.469793
C	3.707690	1.411364	2.464642

C	4.888505	0.714879	2.461189
C	4.888505	-0.714879	2.461189
C	3.707690	-1.411364	2.464642
H	-5.835271	-1.248215	2.450944
H	-3.705497	-2.498698	2.455530
H	-3.705497	2.498698	2.455530
H	-5.835271	1.248215	2.450944
H	-1.234496	-2.498529	2.460042
H	-1.234496	2.498529	2.460042
H	1.234496	-2.498529	2.460042
H	1.234496	2.498529	2.460042
H	3.705497	2.498698	2.455530
H	5.835271	1.248215	2.450944
H	5.835271	-1.248215	2.450944
H	3.705497	-2.498698	2.455530
C	4.886584	0.000000	-1.747135
C	3.704152	0.000000	-1.053478
C	2.448885	0.000000	-1.741523
C	2.450811	0.000000	-3.197270
C	3.711145	0.000000	-3.877329
C	4.890569	0.000000	-3.177352
C	1.235010	0.000000	-3.881684
C	0.000000	0.000000	-3.200638
C	0.000000	0.000000	-1.742692
C	1.232744	0.000000	-1.058386
C	-1.232744	0.000000	-1.058386
C	-2.448885	0.000000	-1.741523
C	-2.450811	0.000000	-3.197270
C	-1.235010	0.000000	-3.881684
C	-3.704152	0.000000	-1.053478
C	-4.886584	0.000000	-1.747135
C	-4.890569	0.000000	-3.177352
C	-3.711145	0.000000	-3.877329
H	5.831493	0.000000	-1.209291
H	3.701412	0.000000	0.031362
H	3.712394	0.000000	-4.965270
H	5.838933	0.000000	-3.709046
H	1.236721	0.000000	-4.970292
H	1.232885	0.000000	0.027257
H	-1.232885	0.000000	0.027257
H	-1.236721	0.000000	-4.970292
H	-3.701412	0.000000	0.031362
H	-5.831493	0.000000	-1.209291
H	-5.838933	0.000000	-3.709046
H	-3.712394	0.000000	-4.965270

134 tetradecahydroanthracene dimer

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.368429	-1.423333	0.000000
C	-1.906281	-0.705995	-1.273115
C	-2.372709	0.764073	-1.275240
C	-1.911417	1.480567	0.000000
C	-2.372709	0.764073	1.275240
C	-1.906281	-0.705995	1.273115
C	-2.368143	-1.430754	2.544681
C	-1.895708	-0.709070	3.815838
C	-2.344266	0.761570	3.820356
C	-1.893181	1.486159	2.542842
C	-2.368143	-1.430754	-2.544681
C	-1.895708	-0.709070	-3.815838
C	-2.344266	0.761570	-3.820356
C	-1.893181	1.486159	-2.542842
H	-1.996678	-2.457831	0.000000
H	-3.468359	-1.478656	0.000000
H	-0.806832	-0.694567	-1.272318
H	-3.475627	0.753806	-1.282695
H	-0.813011	1.532580	0.000000
H	-2.278486	2.516553	0.000000
H	-3.475627	0.753806	1.282695
H	-0.806832	-0.694567	1.272318
H	-2.000137	-2.465651	2.533131
H	-3.467766	-1.480364	2.539623
H	-2.272817	-1.223883	4.708769
H	-0.799314	-0.749716	3.860596
H	-1.951474	1.274798	4.707606
H	-3.441766	0.800591	3.884115
H	-0.795658	1.536142	2.521206
H	-2.259863	2.521437	2.539624
H	-3.467766	-1.480364	-2.539623
H	-2.000137	-2.465651	-2.533131
H	-0.799314	-0.749716	-3.860596
H	-2.272817	-1.223883	-4.708769
H	-3.441766	0.800591	-3.884115
H	-1.951474	1.274798	-4.707606
H	-0.795658	1.536142	-2.521206
H	-2.259863	2.521437	-2.539624
C	1.911417	-1.480567	0.000000
C	2.372709	-0.764073	-1.275240
C	1.906281	0.705995	-1.273115
C	2.368429	1.423333	0.000000

C	1.906281	0.705995	1.273115
C	2.372709	-0.764073	1.275240
C	1.893181	-1.486159	2.542842
C	2.344266	-0.761570	3.820356
C	1.895708	0.709070	3.815838
C	2.368143	1.430754	2.544681
C	2.368143	1.430754	-2.544681
C	1.895708	0.709070	-3.815838
C	2.344266	-0.761570	-3.820356
C	1.893181	-1.486159	-2.542842
H	2.278486	-2.516553	0.000000
H	0.813011	-1.532580	0.000000
H	3.475627	-0.753806	-1.282695
H	0.806832	0.694567	-1.272318
H	3.468359	1.478656	0.000000
H	1.996678	2.457831	0.000000
H	0.806832	0.694567	1.272318
H	3.475627	-0.753806	1.282695
H	2.259863	-2.521437	2.539624
H	0.795658	-1.536142	2.521206
H	1.951474	-1.274798	4.707606
H	3.441766	-0.800591	3.884115
H	2.272817	1.223883	4.708769
H	0.799314	0.749716	3.860596
H	3.467766	1.480364	2.539623
H	2.000137	2.465651	2.533131
H	3.467766	1.480364	-2.539623
H	2.000137	2.465651	-2.533131
H	0.799314	0.749716	-3.860596
H	2.272817	1.223883	-4.708769
H	3.441766	-0.800591	-3.884115
H	1.951474	-1.274798	-4.707606
H	0.795658	-1.536142	-2.521206
H	2.259863	-2.521437	-2.539624

135 octadecahydrotetracene dimer

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.367447	-1.418286	-1.271990
C	-1.905918	-0.701443	-2.545535
C	-2.369628	0.769698	-2.548476
C	-1.909312	1.486881	-1.272842
C	-2.375623	0.769489	0.000000
C	-1.906303	-0.698715	0.000000
C	-2.367447	-1.418286	1.271990

C	-1.905918	-0.701443	2.545535
C	-2.369628	0.769698	2.548476
C	-1.909312	1.486881	1.272842
C	-2.371147	-1.426161	-3.815986
C	-1.899588	-0.706803	-5.088725
C	-2.344234	0.765084	-5.093234
C	-1.888362	1.489090	-3.816949
C	-1.888362	1.489090	3.816949
C	-2.344234	0.765084	5.093234
C	-1.899588	-0.706803	5.088725
C	-2.371147	-1.426161	3.815986
H	-1.994547	-2.452317	-1.271568
H	-3.467287	-1.474656	-1.271664
H	-0.806550	-0.691866	-2.546145
H	-3.472554	0.761231	-2.556800
H	-0.810889	1.538369	-1.270431
H	-2.275826	2.522997	-1.274210
H	-3.478343	0.756293	0.000000
H	-0.806954	-0.686229	0.000000
H	-1.994547	-2.452317	1.271568
H	-3.467287	-1.474656	1.271664
H	-0.806550	-0.691866	2.546145
H	-3.472554	0.761231	2.556800
H	-0.810889	1.538369	1.270431
H	-2.275826	2.522997	1.274210
H	-3.470842	-1.473494	-3.808891
H	-2.005217	-2.461790	-3.804134
H	-0.803481	-0.750658	-5.136182
H	-2.280239	-1.221198	-5.980401
H	-3.441745	0.806935	-5.154769
H	-1.951791	1.277388	-5.981175
H	-2.250742	2.525876	-3.814106
H	-0.790674	1.534042	-3.797019
H	-2.250742	2.525876	3.814106
H	-0.790674	1.534042	3.797019
H	-1.951791	1.277388	5.981175
H	-3.441745	0.806935	5.154769
H	-2.280239	-1.221198	5.980401
H	-0.803481	-0.750658	5.136182
H	-2.005217	-2.461790	3.804134
H	-3.470842	-1.473494	3.808891
C	1.909312	-1.486881	-1.272842
C	2.369628	-0.769698	-2.548476
C	1.905918	0.701443	-2.545535
C	2.367447	1.418286	-1.271990
C	1.906303	0.698715	0.000000

C	2.375623	-0.769489	0.000000
C	1.909312	-1.486881	1.272842
C	2.369628	-0.769698	2.548476
C	1.905918	0.701443	2.545535
C	2.367447	1.418286	1.271990
C	2.371147	1.426161	-3.815986
C	1.899588	0.706803	-5.088725
C	2.344234	-0.765084	-5.093234
C	1.888362	-1.489090	-3.816949
C	2.371147	1.426161	3.815986
C	1.899588	0.706803	5.088725
C	2.344234	-0.765084	5.093234
C	1.888362	-1.489090	3.816949
H	2.275826	-2.522997	-1.274210
H	0.810889	-1.538369	-1.270431
H	3.472554	-0.761231	-2.556800
H	0.806550	0.691866	-2.546145
H	3.467287	1.474656	-1.271664
H	1.994547	2.452317	-1.271568
H	0.806954	0.686229	0.000000
H	3.478343	-0.756293	0.000000
H	2.275826	-2.522997	1.274210
H	0.810889	-1.538369	1.270431
H	3.472554	-0.761231	2.556800
H	0.806550	0.691866	2.546145
H	3.467287	1.474656	1.271664
H	1.994547	2.452317	1.271568
H	3.470842	1.473494	-3.808891
H	2.005217	2.461790	-3.804134
H	0.803481	0.750658	-5.136182
H	2.280239	1.221198	-5.980401
H	3.441745	-0.806935	-5.154769
H	1.951791	-1.277388	-5.981175
H	2.250742	-2.525876	-3.814106
H	0.790674	-1.534042	-3.797019
H	2.005217	2.461790	3.804134
H	3.470842	1.473494	3.808891
H	2.280239	1.221198	5.980401
H	0.803481	0.750658	5.136182
H	1.951791	-1.277388	5.981175
H	3.441745	-0.806935	5.154769
H	2.250742	-2.525876	3.814106
H	0.790674	-1.534042	3.797019

136 [4]-ladderane dimer (C_s)

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-0.801227	2.166564	2.586022
C	0.675185	1.653800	2.591715
C	-0.531636	2.975215	1.284092
C	0.967068	2.439526	1.281013
C	-0.829618	2.175095	0.000000
C	0.682328	1.627853	0.000000
C	-0.531636	2.975215	-1.284092
C	0.967068	2.439526	-1.281013
C	-0.801227	2.166564	-2.586022
C	0.675185	1.653800	-2.591715
H	-1.586027	1.397748	2.494474
H	-1.039425	2.802308	3.452198
H	1.250057	2.026974	3.452730
H	0.817418	0.564254	2.521102
H	-0.816457	4.039529	1.282612
H	1.860379	3.084232	1.266617
H	-1.740887	1.551767	0.000000
H	0.976454	0.567638	0.000000
H	-0.816457	4.039529	-1.282612
H	1.860379	3.084232	-1.266617
H	-1.039425	2.802308	-3.452198
H	-1.586027	1.397748	-2.494474
H	0.817418	0.564254	-2.521102
H	1.250057	2.026974	-3.452730
C	-0.920582	-2.202624	-2.598437
C	0.537761	-2.763895	-2.581232
C	-0.659472	-1.445135	-1.270974
C	0.847936	-1.959304	-1.284611
C	-0.930646	-2.278008	0.000000
C	0.597346	-2.772301	0.000000
C	-0.659472	-1.445135	1.270974
C	0.847936	-1.959304	1.284611
C	-0.920582	-2.202624	2.598437
C	0.537761	-2.763895	2.581232
H	-1.098301	-1.520629	-3.444039
H	-1.737119	-2.942734	-2.565349
H	0.632115	-3.854738	-2.463445
H	1.137036	-2.452399	-3.450576
H	-0.959986	-0.389294	-1.224048
H	1.735520	-1.306204	-1.299334
H	-1.816601	-2.936132	0.000000
H	0.930778	-3.824717	0.000000
H	-0.959986	-0.389294	1.224048
H	1.735520	-1.306204	1.299334

H	-1.737119	-2.942734	2.565349
H	-1.098301	-1.520629	3.444039
H	1.137036	-2.452399	3.450576
H	0.632115	-3.854738	2.463445

137 [5]-ladderane dimer (C_i)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.577236	0.903828	0.136689
C	3.569904	0.857847	-1.425746
C	2.508351	2.034441	0.121273
C	2.508956	1.995433	-1.470216
C	1.062939	1.496618	0.140049
C	1.059086	1.470933	-1.464016
C	0.002292	2.613145	0.121883
C	0.013842	2.604274	-1.479804
C	-1.427475	2.026407	0.115384
C	-1.433766	2.080074	-1.476174
C	-2.487638	3.226325	-1.405583
C	-2.555734	3.087059	0.149345
H	3.266576	-0.016913	0.655721
H	4.544643	1.228744	0.548413
H	4.535149	1.146443	-1.868571
H	3.246950	-0.090368	-1.886116
H	2.711056	2.933097	0.725444
H	2.722134	2.860186	-2.118737
H	0.859985	0.631566	0.790415
H	0.843937	0.590346	-2.094047
H	0.184602	3.497489	0.756718
H	0.232175	3.474480	-2.122980
H	-1.570579	1.114555	0.710210
H	-1.665402	1.226231	-2.133353
H	-2.111839	4.192641	-1.778889
H	-3.436053	2.999691	-1.915136
H	-2.344140	3.991002	0.743263
H	-3.514083	2.660694	0.485598
C	2.487638	-3.226325	1.405583
C	2.555734	-3.087059	-0.149345
C	1.433766	-2.080074	1.476174
C	1.427475	-2.026407	-0.115384
C	-0.013842	-2.604274	1.479804
C	-0.002292	-2.613145	-0.121883
C	-1.059086	-1.470933	1.464016
C	-1.062939	-1.496618	-0.140049
C	-2.508956	-1.995433	1.470216

C	-2.508351	-2.034441	-0.121273
C	-3.577236	-0.903828	-0.136689
C	-3.569904	-0.857847	1.425746
H	2.111839	-4.192641	1.778889
H	3.436053	-2.999691	1.915136
H	3.514083	-2.660694	-0.485598
H	2.344140	-3.991002	-0.743263
H	1.665402	-1.226231	2.133353
H	1.570579	-1.114555	-0.710210
H	-0.232175	-3.474480	2.122980
H	-0.184602	-3.497489	-0.756718
H	-0.843937	-0.590346	2.094047
H	-0.859985	-0.631566	-0.790415
H	-2.722134	-2.860186	2.118737
H	-2.711056	-2.933097	-0.725444
H	-3.266576	0.016913	-0.655721
H	-4.544643	-1.228744	-0.548413
H	-3.246950	0.090368	1.886116
H	-4.535149	-1.146443	1.868571

138 octadecane dimer

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	20.737000	13.092000	2.121000
C	20.064000	11.721000	1.997000
C	18.539000	11.784000	2.146000
C	17.856000	10.417000	2.022000
C	16.330000	10.486000	2.157000
C	15.644000	9.122000	2.026000
C	14.117000	9.196000	2.146000
C	13.427000	7.835000	2.005000
C	11.900000	7.916000	2.116000
C	11.204000	6.557000	1.972000
C	9.678000	6.644000	2.084000
C	8.976000	5.288000	1.945000
C	7.451000	5.379000	2.067000
C	6.746000	4.024000	1.939000
C	5.222000	4.116000	2.078000
C	4.516000	2.760000	1.964000
C	2.993000	2.850000	2.120000
C	2.297000	1.489000	2.014000
H	20.542000	13.536000	3.104000
H	21.822000	13.016000	1.994000
H	20.357000	13.784000	1.361000
H	20.311000	11.278000	1.023000

H	20.472000	11.042000	2.758000
H	18.289000	12.227000	3.120000
H	18.130000	12.463000	1.384000
H	18.113000	9.971000	1.051000
H	18.257000	9.741000	2.789000
H	16.073000	10.929000	3.130000
H	15.930000	11.167000	1.393000
H	15.909000	8.675000	1.057000
H	16.035000	8.443000	2.797000
H	13.852000	9.638000	3.117000
H	13.728000	9.880000	1.379000
H	13.696000	7.390000	1.037000
H	13.810000	7.152000	2.777000
H	11.631000	8.358000	3.086000
H	11.518000	8.601000	1.347000
H	11.472000	6.113000	1.004000
H	11.585000	5.872000	2.743000
H	9.412000	7.089000	3.053000
H	9.297000	7.330000	1.314000
H	9.237000	4.841000	0.975000
H	9.359000	4.602000	2.714000
H	7.194000	5.829000	3.037000
H	7.066000	6.063000	1.298000
H	6.995000	3.575000	0.968000
H	7.137000	3.340000	2.706000
H	4.976000	4.570000	3.049000
H	4.828000	4.796000	1.311000
H	4.754000	2.307000	0.991000
H	4.917000	2.079000	2.728000
H	2.758000	3.307000	3.091000
H	2.593000	3.527000	1.354000
H	1.211000	1.588000	2.119000
H	2.500000	1.019000	1.045000
H	2.651000	0.807000	2.796000
C	4.969000	4.711000	-2.053000
C	4.286000	3.344000	-2.177000
C	2.761000	3.407000	-2.028000
C	2.088000	2.036000	-2.152000
C	6.494000	4.642000	-2.189000
C	7.181000	6.007000	-2.057000
C	8.707000	5.932000	-2.177000
C	9.398000	7.293000	-2.036000
C	10.925000	7.212000	-2.147000
C	11.620000	8.571000	-2.003000
C	13.147000	8.484000	-2.115000
C	13.848000	9.841000	-1.976000

C	15.373000	9.749000	-2.098000
C	16.078000	11.105000	-1.970000
C	17.602000	11.012000	-2.110000
C	18.308000	12.368000	-1.995000
C	19.831000	12.278000	-2.151000
C	20.527000	13.639000	-2.046000
H	4.712000	5.157000	-1.082000
H	4.567000	5.387000	-2.821000
H	4.536000	2.901000	-3.152000
H	4.694000	2.665000	-1.416000
H	2.514000	3.850000	-1.054000
H	2.353000	4.086000	-2.789000
H	1.003000	2.112000	-2.026000
H	2.283000	1.592000	-3.136000
H	2.468000	1.344000	-1.393000
H	6.751000	4.200000	-3.162000
H	6.894000	3.961000	-1.425000
H	6.916000	6.453000	-1.089000
H	6.789000	6.685000	-2.828000
H	8.972000	5.490000	-3.149000
H	9.096000	5.248000	-1.410000
H	9.128000	7.738000	-1.069000
H	9.015000	7.976000	-2.808000
H	11.194000	6.770000	-3.117000
H	11.307000	6.527000	-1.378000
H	11.352000	9.016000	-1.035000
H	11.240000	9.256000	-2.774000
H	13.412000	8.039000	-3.084000
H	13.527000	7.799000	-1.345000
H	13.588000	10.287000	-1.006000
H	13.465000	10.526000	-2.745000
H	15.630000	9.299000	-3.068000
H	15.759000	9.066000	-1.329000
H	15.829000	11.554000	-0.999000
H	15.687000	11.788000	-2.737000
H	17.848000	10.558000	-3.080000
H	17.996000	10.332000	-1.342000
H	18.070000	12.822000	-1.023000
H	17.907000	13.049000	-2.760000
H	20.066000	11.821000	-3.122000
H	20.231000	11.601000	-1.385000
H	21.613000	13.541000	-2.151000
H	20.173000	14.321000	-2.828000
H	20.324000	14.109000	-1.076000