

Structures Optimized at the DFT-D level. Atomic coordinates are in Å .
Each heading is taken from the appropriate database. The next line contains the
calculated DFT-D energy (au).

1 adenine_thymine_wc c1 -16.37

-921.5908367288115

1	7	0	0.934468	-0.006651	-0.388326
2	6	0	1.682042	-0.005946	0.749056
3	6	0	3.092550	0.000974	0.598851
4	6	0	3.582010	0.004857	-0.718190
5	7	0	2.861362	0.003089	-1.855716
6	6	0	1.545731	-0.002511	-1.595708
7	7	0	4.131143	0.005419	1.525087
8	6	0	5.223644	0.011208	0.785308
9	7	0	4.959354	0.010900	-0.577270
10	7	0	1.059210	-0.015567	1.945925
11	1	0	0.868971	-0.003475	-2.449469
12	1	0	6.238582	0.015855	1.163998
13	1	0	5.632191	0.014716	-1.333552
14	1	0	0.033553	-0.000908	2.001810
15	1	0	1.617822	0.002103	2.787902
16	7	0	-3.921991	0.008809	-1.524387
17	6	0	-4.625474	0.011996	-0.336600
18	6	0	-4.009926	0.011210	0.875539
19	6	0	-2.542419	0.007504	0.896989
20	7	0	-1.908084	0.002545	-0.350767
21	6	0	-2.519312	0.003851	-1.596967
22	6	0	-4.753842	0.014721	2.184097
23	8	0	-1.873297	0.008544	1.946721
24	8	0	-1.916711	0.000008	-2.667199
25	1	0	-4.404782	0.010096	-2.414969
26	1	0	-0.850957	-0.003547	-0.358465
27	1	0	-5.707989	0.015127	-0.437616
28	1	0	-4.490216	-0.864873	2.785129
29	1	0	-4.485578	0.894301	2.783092
30	1	0	-5.837683	0.017360	2.021126

2 adenine_thymine_stack c1 -12.23

-921.5840088230138

1	7	0	0.286379	2.522654	-0.582845
2	6	0	-1.098212	2.528765	-0.548501
3	1	0	-1.675066	3.099487	-1.265413
4	7	0	-1.600303	1.783806	0.418905
5	6	0	-0.482095	1.244550	1.046591
6	6	0	-0.331427	0.325666	2.112745
7	7	0	-1.398788	-0.212255	2.772403
8	1	0	-1.199881	-1.015001	3.358554
9	1	0	-2.284573	-0.227341	2.278388
10	7	0	0.918927	-0.021914	2.496276

11	6	0	1.966604	0.493532	1.821276
12	1	0	2.948741	0.174447	2.170098
13	7	0	1.961042	1.335592	0.770527
14	6	0	0.706797	1.683899	0.435006
15	1	0	0.868971	2.922783	-1.307667
16	7	0	1.276244	-0.700974	-1.982966
17	6	0	1.401944	-1.625564	-0.961687
18	1	0	2.420562	-1.933842	-0.744840
19	6	0	0.336956	-2.107375	-0.270802
20	6	0	0.464681	-3.096846	0.854719
21	1	0	0.178533	-2.634614	1.807125
22	1	0	-0.198085	-3.956024	0.694976
23	1	0	1.496066	-3.454583	0.946837
24	6	0	-0.997841	-1.602755	-0.613821
25	8	0	-2.044083	-1.903458	-0.037107
26	7	0	-1.023847	-0.689670	-1.700677
27	1	0	-1.928478	-0.272349	-1.905048
28	6	0	0.060612	-0.144901	-2.381413
29	8	0	-0.028566	0.736993	-3.233778
30	1	0	2.100872	-0.305274	-2.418011

101 ammonia_dimer c2h -3.17
-113.1267158050666

1	7	0	-1.626402	-0.042050	0.000719
2	1	0	-2.213024	0.138452	-0.816222
3	1	0	-2.208706	0.144747	0.819332
4	1	0	-0.891805	0.670449	-0.003829
5	7	0	1.626402	0.042050	0.000719
6	1	0	2.213024	-0.138452	-0.816222
7	1	0	0.891805	-0.670449	-0.003829
8	1	0	2.208706	-0.144747	0.819332

102 water_dimer cs -5.02
-152.9047364937420

1	8	0	-1.544710	-0.123132	0.000008
2	1	0	-1.942615	0.761673	-0.000012
3	1	0	-0.579199	0.043846	0.000005
4	8	0	1.379082	0.139370	0.000002
5	1	0	1.656959	-0.384532	-0.770032
6	1	0	1.656961	-0.384542	0.770028

103 methane_dimer d3d -0.53
-81.00316164283218

1	6	0	0.000000	-0.000106	1.858399
2	1	0	-0.893077	0.515492	1.491627
3	1	0	0.893077	0.515492	1.491627
4	1	0	0.000000	-1.031427	1.491937

5	1	0	0.000000	0.000138	2.953194
6	6	0	0.000000	0.000106	-1.858399
7	1	0	0.000000	-0.000138	-2.953194
8	1	0	-0.893077	-0.515492	-1.491627
9	1	0	0.893077	-0.515492	-1.491627
10	1	0	0.000000	1.031427	-1.491937

104 ethene_dimer d2d -1.51
-157.1561258906295

1	6	0	-0.471682	-0.471682	-1.856202
2	6	0	0.471682	0.471682	-1.856202
3	1	0	-0.873693	-0.873693	-0.928005
4	1	0	0.873693	0.873693	-0.928005
5	1	0	-0.875393	-0.875393	-2.783109
6	1	0	0.875393	0.875393	-2.783109
7	6	0	-0.471682	0.471682	1.856202
8	6	0	0.471682	-0.471682	1.856202
9	1	0	-0.873693	0.873693	0.928005
10	1	0	0.873693	-0.873693	0.928005
11	1	0	-0.875393	0.875393	2.783108
12	1	0	0.875393	-0.875393	2.783108

105 ethene_ethine c2v -1.53
-155.911169779353

1	6	0	0.000000	-0.667477	-2.127521
2	6	0	0.000000	0.667477	-2.127521
3	1	0	0.927413	-1.237523	-2.128333
4	1	0	-0.927413	-1.237523	-2.128333
5	1	0	-0.927413	1.237523	-2.128333
6	1	0	0.927413	1.237523	-2.128333
7	6	0	0.000000	0.000000	2.903840
8	6	0	0.000000	0.000000	1.697252
9	1	0	0.000000	0.000000	0.627022
10	1	0	0.000000	0.000000	3.971226

106 formic_acid_dimer c2h -18.61
-379.657548107064

1	6	0	-1.903386	-0.189642	-0.000104
2	8	0	-1.496656	1.072788	0.001438
3	8	0	-1.189860	-1.193588	-0.002044
4	1	0	-3.002592	-0.258486	0.000546
5	1	0	-0.482665	1.117673	0.000164
6	6	0	1.903386	0.189642	-0.000104
7	8	0	1.496656	-1.072788	0.001438
8	8	0	1.189860	1.193588	-0.002044
9	1	0	3.002592	0.258486	0.000546
10	1	0	0.482665	-1.117673	0.000164

107 formamide_dimer c2h -15.96
-339.8823605856300

1	6	0	-2.041336	0.054314	0.000000
2	8	0	-1.472856	1.156071	0.000005
3	7	0	-1.422484	-1.145304	0.000000
4	1	0	-1.975118	-1.992939	-0.000004
5	1	0	-0.390017	-1.209958	0.000002
6	1	0	-3.148271	-0.014151	-0.000003
7	6	0	2.041345	-0.054286	0.000000
8	8	0	1.472876	-1.156070	0.000006
9	7	0	1.422478	1.145295	0.000000
10	1	0	1.975096	1.992932	-0.000004
11	1	0	0.390016	1.209935	0.000003
12	1	0	3.148269	0.014162	-0.000004

108 benzene_water cs -3.28
-308.6805347319094

1	6	0	0.709601	-0.615890	-1.213604
2	6	0	0.472710	0.764080	-1.213784
3	6	0	0.354907	1.454355	-0.000021
4	6	0	0.472649	0.764079	1.213754
5	6	0	0.709547	-0.615915	1.213576
6	6	0	0.829280	-1.305608	-0.000025
7	1	0	0.797715	-1.152598	-2.155138
8	1	0	0.376146	1.299190	-2.155351
9	1	0	0.172818	2.526630	-0.000021
10	1	0	0.376055	1.299181	2.155343
11	1	0	0.797637	-1.152638	2.155120
12	1	0	1.015620	-2.377206	-0.000023
13	8	0	-2.686884	-0.509090	0.000028
14	1	0	-2.025309	-1.220236	0.000101
15	1	0	-2.138616	0.293394	0.000037

109 benzene_ammonia cs -2.35
-288.7909205162225

1	6	0	-0.756974	0.536868	-1.212747
2	6	0	-1.449305	0.430413	0.000000
3	6	0	-0.756974	0.536868	1.212747
4	6	0	0.627427	0.749294	1.212646
5	6	0	1.319605	0.855630	0.000000
6	6	0	0.627427	0.749294	-1.212646
7	1	0	-1.294111	0.450068	-2.154279
8	1	0	-2.522880	0.258580	0.000000
9	1	0	-1.294111	0.450068	2.154279
10	1	0	1.165107	0.829614	2.154628
11	1	0	2.395005	1.017830	0.000000

12	1	0	1.165107	0.829614	-2.154628
13	7	0	0.220940	-2.973747	0.000000
14	1	0	0.805702	-3.164415	-0.816288
15	1	0	0.805702	-3.164415	0.816288
16	1	0	0.056871	-1.965075	0.000000

110 benzene_methane c3 -1.50
-272.7298243419870

1	6	0	1.399741	0.036461	-0.638780
2	6	0	0.731430	-1.193960	-0.638755
3	6	0	-0.668304	-1.230447	-0.638772
4	6	0	-1.399721	-0.036460	-0.638771
5	6	0	-0.731430	1.193986	-0.638774
6	6	0	0.668292	1.230442	-0.638802
7	1	0	2.486953	0.064764	-0.635809
8	1	0	1.299565	-2.121354	-0.635799
9	1	0	-1.187397	-2.186154	-0.635826
10	1	0	-2.486933	-0.064770	-0.635793
11	1	0	-1.299552	2.121387	-0.635822
12	1	0	1.187375	2.186156	-0.635881
13	6	0	-0.000003	-0.000006	3.093346
14	1	0	0.591694	0.845240	3.460792
15	1	0	-1.027866	0.089780	3.460768
16	1	0	0.000000	0.000001	2.000198
17	1	0	0.436155	-0.935065	3.460763

111 benzene_dimer c2v -2.74
-464.4574911653282

1	6	0	0.000000	-0.000002	1.123964
2	6	0	-0.000008	-1.211590	1.825693
3	6	0	-0.000008	-1.212631	3.226116
4	6	0	0.000000	0.000002	3.926758
5	6	0	0.000008	1.212632	3.226112
6	6	0	0.000008	1.211587	1.825690
7	1	0	0.000000	-0.000003	0.039112
8	1	0	-0.000014	-2.152692	1.280126
9	1	0	-0.000014	-2.154636	3.770338
10	1	0	0.000000	0.000003	5.014593
11	1	0	0.000014	2.154639	3.770331
12	1	0	0.000014	2.152687	1.280120
13	6	0	-1.400458	-0.000004	-2.527030
14	6	0	-0.700199	1.212621	-2.527436
15	6	0	0.700192	1.212625	-2.527436
16	6	0	1.400458	0.000005	-2.527030
17	6	0	0.700200	-1.212620	-2.527440
18	6	0	-0.700192	-1.212625	-2.527440
19	1	0	-2.487887	-0.000007	-2.521245
20	1	0	-1.244181	2.154347	-2.523814

21	1	0	1.244168	2.154355	-2.523814
22	1	0	2.487887	0.000008	-2.521245
23	1	0	1.244182	-2.154347	-2.523822
24	1	0	-1.244168	-2.154355	-2.523822

112 benzene_dimer c2h -2.73
-464.4572090993442

1	6	0	-1.049034	-1.429535	0.000000
2	6	0	-1.457650	-0.861287	1.210936
3	6	0	-1.457650	-0.861287	-1.210936
4	6	0	-2.271618	0.277434	1.212191
5	6	0	-2.677497	0.848513	0.000000
6	6	0	-2.271618	0.277434	-1.212191
7	1	0	-1.128647	-1.295508	-2.152006
8	1	0	-2.583768	0.722359	-2.154635
9	1	0	-3.307595	1.735475	0.000000
10	1	0	-2.583768	0.722359	2.154635
11	1	0	-1.128647	-1.295508	2.152006
12	1	0	-0.396079	-2.298236	0.000000
13	6	0	1.049034	1.429535	0.000000
14	6	0	1.457650	0.861287	-1.210936
15	6	0	1.457650	0.861287	1.210936
16	6	0	2.271618	-0.277434	-1.212191
17	6	0	2.677497	-0.848513	0.000000
18	6	0	2.271618	-0.277434	1.212191
19	1	0	0.396079	2.298236	0.000000
20	1	0	1.128647	1.295508	2.152006
21	1	0	2.583768	-0.722359	2.154635
22	1	0	3.307595	-1.735475	0.000000
23	1	0	2.583768	-0.722359	-2.154635
24	1	0	1.128647	1.295508	-2.152006

113 indole_benzene_t-shape c1 -7.03
-596.0396575189886

1	6	0	2.518507	1.641396	-0.000904
2	6	0	2.756849	0.982311	-1.213875
3	6	0	3.232135	-0.335541	-1.212908
4	6	0	3.469267	-0.993737	0.001438
5	6	0	3.230396	-0.334012	1.214622
6	6	0	2.754904	0.983780	1.213235
7	1	0	2.145246	2.662423	-0.001658
8	1	0	2.565682	1.491156	-2.155287
9	1	0	3.411118	-0.849123	-2.154439
10	1	0	3.835889	-2.017691	0.002325
11	1	0	3.408809	-0.846189	2.157092
12	1	0	2.562863	1.494046	2.153756
13	1	0	0.756970	-0.547298	0.000194
14	7	0	-0.205687	-0.852125	-0.000155

15	6	0	-0.625698	-2.174060	-0.002592
16	6	0	-2.002653	-2.220366	-0.002218
17	6	0	-2.472535	-0.860708	-0.000322
18	6	0	-1.312483	-0.020868	0.000127
19	6	0	-1.399806	1.377934	0.000070
20	6	0	-2.674484	1.943576	0.001464
21	6	0	-3.834751	1.134727	0.002708
22	6	0	-3.745454	-0.255573	0.001235
23	1	0	0.100383	-2.975963	-0.003021
24	1	0	-2.606315	-3.118495	-0.002759
25	1	0	-0.505837	1.996703	-0.004900
26	1	0	-2.778821	3.026020	0.001295
27	1	0	-4.812497	1.610880	0.004271
28	1	0	-4.646298	-0.865829	0.001205

114 indole_benzene_stack c1 -8.12
-596.0382361012972

1	6	0	0.005439	1.469635	-1.447052
2	6	0	-1.249604	0.908582	-1.705637
3	6	0	-1.349413	-0.263932	-2.462520
4	6	0	-0.193313	-0.876477	-2.961275
5	6	0	1.063073	-0.312333	-2.704697
6	6	0	1.161638	0.861628	-1.948641
7	1	0	0.084103	2.368110	-0.841421
8	1	0	-2.144529	1.371644	-1.298700
9	1	0	-2.324783	-0.704708	-2.655733
10	1	0	-0.271113	-1.787560	-3.551022
11	1	0	1.961768	-0.784635	-3.096869
12	1	0	2.136027	1.294100	-1.736441
13	1	0	-2.961301	0.906302	2.427911
14	6	0	-2.045045	0.439930	2.073269
15	6	0	-0.822777	1.074349	2.283724
16	1	0	-0.779240	2.032186	2.798189
17	6	0	0.355864	0.459405	1.816751
18	6	0	1.749183	0.816204	1.826572
19	1	0	2.191973	1.703072	2.260731
20	6	0	2.431818	-0.191327	1.183463
21	7	0	1.538048	-1.178774	0.790450
22	6	0	0.253523	-0.799258	1.145408
23	6	0	-0.971883	-1.442115	0.938225
24	1	0	-1.031147	-2.393482	0.414900
25	6	0	-2.119017	-0.806370	1.409170
26	1	0	-3.088962	-1.274260	1.259280
27	1	0	1.763337	-1.950083	0.179258
28	1	0	3.488458	-0.296703	0.977043

117 pyrazine_dimer cs -4.42
-528.6606379887392

1	6	0	-1.274561	-1.251304	-0.699738
2	6	0	-1.274561	-1.251304	0.699738
3	7	0	-0.274084	-1.795116	1.416197
4	6	0	0.727039	-2.333433	0.700395
5	6	0	0.727039	-2.333433	-0.700395
6	7	0	-0.274084	-1.795116	-1.416197
7	1	0	-2.097136	-0.801363	-1.255029
8	1	0	-2.097136	-0.801363	1.255029
9	1	0	1.554981	-2.773974	1.255698
10	1	0	1.554981	-2.773974	-1.255698
11	6	0	-0.323829	2.157912	1.137656
12	6	0	0.871619	1.428625	1.137762
13	7	0	1.483503	1.057032	0.000000
14	6	0	0.871619	1.428625	-1.137762
15	6	0	-0.323829	2.157912	-1.137656
16	7	0	-0.935465	2.531451	0.000000
17	1	0	-0.800287	2.443469	2.075591
18	1	0	1.338438	1.127767	2.075078
19	1	0	1.338438	1.127767	-2.075078
20	1	0	-0.800287	2.443469	-2.075591

118 2-pyridoxine_2-aminopyridine c1 -16.71

-627.2282627735380

1	8	0	-1.437437	-1.952892	-0.156766
2	7	0	-1.459969	0.348377	0.036095
3	6	0	-4.205069	0.386909	0.023396
4	6	0	-3.481988	1.606560	0.138586
5	6	0	-2.110127	1.540808	0.140206
6	6	0	-2.107593	-0.898877	-0.074430
7	6	0	-3.553430	-0.819417	-0.079969
8	1	0	-5.293325	0.411389	0.018241
9	1	0	-3.986630	2.562332	0.222571
10	1	0	-1.475438	2.419025	0.223602
11	1	0	-4.095457	-1.756254	-0.166641
12	1	0	-0.410176	0.339355	0.031632
13	7	0	1.435398	0.363838	0.016166
14	6	0	2.131985	-0.801508	0.112271
15	6	0	3.554981	-0.807876	0.075441
16	6	0	4.234077	0.391484	-0.057417
17	6	0	3.512899	1.595417	-0.155363
18	6	0	2.125163	1.515412	-0.113849
19	1	0	4.092968	-1.750255	0.153054
20	1	0	5.321478	0.397413	-0.087334
21	1	0	4.011431	2.553647	-0.261678
22	1	0	1.519777	2.419175	-0.190672
23	7	0	1.412780	-1.949223	0.277841
24	1	0	1.894822	-2.832477	0.185104
25	1	0	0.393809	-1.948868	0.113443

121 phenol_dimer c1 -7.05

-614.9664823886418

1	6	0	-2.043129	0.715081	-0.139728
2	8	0	-1.355428	1.840587	-0.537926
3	1	0	-0.496142	1.889968	-0.069174
4	6	0	-1.544945	-0.183662	0.820762
5	6	0	-2.295066	-1.311049	1.173700
6	6	0	-3.539148	-1.555406	0.581857
7	6	0	-4.029553	-0.654689	-0.373827
8	6	0	-3.291567	0.474273	-0.737247
9	1	0	-0.577107	-0.003618	1.282907
10	1	0	-1.899444	-2.001662	1.916011
11	1	0	-4.117768	-2.432670	0.859485
12	1	0	-4.995448	-0.831586	-0.842283
13	1	0	-3.667610	1.175467	-1.478826
14	8	0	1.338274	1.890357	0.502727
15	6	0	2.083750	0.762960	0.150279
16	1	0	1.682306	2.266365	1.329993
17	6	0	1.696232	0.079259	-1.008378
18	6	0	2.410426	-1.057466	-1.396083
19	6	0	3.499863	-1.511048	-0.641255
20	6	0	3.874021	-0.817743	0.515011
21	6	0	3.167485	0.321452	0.917999
22	1	0	0.844532	0.432609	-1.583555
23	1	0	2.108978	-1.592231	-2.293851
24	1	0	4.049455	-2.396102	-0.950023
25	1	0	4.716565	-1.159968	1.111048
26	1	0	3.459792	0.858717	1.820357

122 uracil_dimer_stack c2 -10.12

-829.7961981650420

1	7	0	2.115815	-1.242370	-0.079836
2	6	0	2.098457	-0.741142	-1.362325
3	1	0	2.377208	-1.445344	-2.139983
4	6	0	1.741811	0.540077	-1.627380
5	1	0	1.724081	0.923284	-2.639890
6	6	0	1.303127	1.414538	-0.547459
7	8	0	0.839238	2.548713	-0.672389
8	7	0	1.420600	0.827038	0.744485
9	1	0	1.056103	1.372521	1.524091
10	6	0	1.715221	-0.504083	1.043645
11	8	0	1.622279	-0.995582	2.161366
12	1	0	2.227949	-2.237280	0.079671
13	7	0	-2.115895	1.242345	-0.079815
14	6	0	-2.098492	0.741123	-1.362307
15	1	0	-2.377276	1.445311	-2.139966
16	6	0	-1.741765	-0.540075	-1.627365
17	1	0	-1.724000	-0.923278	-2.639875
18	6	0	-1.303043	-1.414516	-0.547442

19	8	0	-0.839082	-2.548661	-0.672372
20	7	0	-1.420565	-0.827027	0.744502
21	1	0	-1.056043	-1.372492	1.524111
22	6	0	-1.715268	0.504075	1.043665
23	8	0	-1.622370	0.995576	2.161391
24	1	0	-2.228091	2.237250	0.079693

123 uracil_dimer_hb c2h -20.65
-829.8111814028562

1	8	0	-1.487237	1.017761	-0.000009
2	6	0	-0.644277	1.932214	-0.000007
3	7	0	0.721600	1.702395	-0.000001
4	6	0	1.645274	2.724755	0.000007
5	6	0	1.286261	4.033914	0.000008
6	6	0	-0.123470	4.403638	0.000001
7	7	0	-0.998144	3.269531	-0.000007
8	8	0	-0.590791	5.537866	0.000000
9	1	0	2.025442	4.825139	0.000013
10	1	0	1.030387	0.712044	-0.000005
11	1	0	-1.995558	3.469549	-0.000011
12	1	0	2.682069	2.401331	0.000011
13	8	0	1.487237	-1.017761	-0.000012
14	6	0	0.644277	-1.932214	-0.000007
15	7	0	-0.721600	-1.702395	0.000000
16	6	0	-1.645274	-2.724755	0.000007
17	6	0	-1.286261	-4.033914	0.000008
18	6	0	0.123470	-4.403638	0.000002
19	7	0	0.998144	-3.269531	-0.000007
20	8	0	0.590791	-5.537866	0.000002
21	1	0	-2.025442	-4.825139	0.000012
22	1	0	-1.030387	-0.712044	-0.000003
23	1	0	1.995558	-3.469549	-0.000012
24	1	0	-2.682069	-2.401331	0.000010

128 benzene_hcn cs -4.46
-325.6752866133132

1	6	0	-0.713053	-1.013282	1.213406
2	6	0	-1.413010	-0.987237	0.000000
3	6	0	-0.713053	-1.013282	-1.213406
4	6	0	0.687177	-1.065285	-1.213593
5	6	0	1.387460	-1.091244	0.000000
6	6	0	0.687177	-1.065285	1.213593
7	1	0	-1.256233	-0.990005	2.155013
8	1	0	-2.499406	-0.943397	0.000000
9	1	0	-1.256233	-0.990005	-2.155013
10	1	0	1.230564	-1.083072	-2.155235
11	1	0	2.474125	-1.129527	0.000000
12	1	0	1.230564	-1.083072	2.155235

13	7	0	-0.005393	3.624926	0.000000
14	6	0	0.074940	2.469776	0.000000
15	1	0	0.149964	1.398505	0.000000

G...C WC

-937.6619956858455

1	6	0	-1.062336	-0.068023	2.982367
2	7	0	-0.891703	-0.088065	4.395776
3	6	0	0.339396	-0.046217	4.985870
4	6	0	1.463798	0.019269	4.222103
5	6	0	1.289577	0.042150	2.786993
6	7	0	0.067174	0.003071	2.221258
7	8	0	-2.216972	-0.115751	2.525884
8	7	0	2.353327	0.105216	1.968875
9	1	0	-1.740134	-0.139826	4.948483
10	1	0	0.360948	-0.068611	6.071465
11	1	0	2.447488	0.051594	4.676849
12	1	0	3.284947	0.121759	2.360020
13	1	0	2.236229	0.092886	0.931496
14	8	0	2.052423	0.036959	-0.803561
15	6	0	0.964943	0.035440	-1.417704
16	7	0	-0.256071	0.084455	-0.695210
17	6	0	-1.522684	0.087300	-1.247371
18	7	0	-1.747257	0.032276	-2.560338
19	6	0	-0.603013	-0.013563	-3.279600
20	6	0	0.731323	-0.013494	-2.830852
21	7	0	1.617652	-0.070844	-3.902637
22	6	0	0.848537	-0.104607	-4.967992
23	7	0	-0.510419	-0.073434	-4.654948
24	7	0	-2.570358	0.186500	-0.383110
25	1	0	-0.163600	0.093051	0.339769
26	1	0	1.189796	-0.151871	-5.994996
27	1	0	-1.292365	-0.086323	-5.297434
28	1	0	-3.486756	0.035588	-0.782401
29	1	0	-2.447268	0.039711	0.625744

mG...mC WC

-1016.260346305432

1	6	0	-0.831540	-0.033239	3.016716
2	7	0	-0.667875	-0.063766	4.441514
3	6	0	0.584033	-0.030134	4.987871
4	6	0	1.702470	0.031485	4.211464
5	6	0	1.518273	0.060114	2.783940
6	7	0	0.286117	0.032790	2.241755
7	8	0	-1.989595	-0.069064	2.560963
8	7	0	2.570444	0.117787	1.948318
9	6	0	-1.883297	-0.132426	5.270124
10	1	0	0.639993	-0.056381	6.072726

11	1	0	2.688691	0.055593	4.661901
12	1	0	3.507811	0.119844	2.325419
13	1	0	2.438247	0.098509	0.913327
14	1	0	-2.450934	-1.037090	5.030264
15	1	0	-2.521976	0.734219	5.072295
16	1	0	-1.593884	-0.145823	6.324620
17	8	0	2.244292	0.036737	-0.820511
18	6	0	1.148165	0.043141	-1.419740
19	7	0	-0.062424	0.099593	-0.678333
20	6	0	-1.336766	0.115070	-1.211924
21	7	0	-1.580829	0.064790	-2.521455
22	6	0	-0.446992	0.009490	-3.259343
23	6	0	0.893599	-0.002485	-2.828652
24	7	0	1.760461	-0.065078	-3.913440
25	6	0	0.968505	-0.090203	-4.963141
26	7	0	-0.388700	-0.047519	-4.637755
27	7	0	-2.371192	0.219811	-0.332892
28	1	0	0.044884	0.106115	0.355253
29	1	0	1.287684	-0.138373	-5.998207
30	6	0	-1.528632	-0.059448	-5.551020
31	1	0	-3.295440	0.088784	-0.720196
32	1	0	-2.236914	0.088274	0.676897
33	1	0	-2.156828	-0.938547	-5.367934
34	1	0	-2.137780	0.840641	-5.411956
35	1	0	-1.153558	-0.089117	-6.578147

A...T WC

-921.5908305014768

1	7	0	0.935439	-0.026405	-0.384667
2	6	0	1.684224	-0.021900	0.751607
3	6	0	3.094556	-0.002745	0.599750
4	6	0	3.582376	0.007756	-0.717937
5	7	0	2.860352	0.002985	-1.854619
6	6	0	1.545174	-0.013605	-1.592887
7	7	0	4.133940	0.008951	1.524953
8	6	0	5.225496	0.025437	0.783649
9	7	0	4.959822	0.025237	-0.578546
10	7	0	1.063261	-0.041006	1.949493
11	1	0	0.867419	-0.016709	-2.445889
12	1	0	6.240767	0.038386	1.161273
13	1	0	5.631768	0.036575	-1.335594
14	1	0	0.038001	-0.021434	2.006781
15	1	0	1.622877	-0.007512	2.790363
16	7	0	-3.923625	0.013513	-1.525641
17	6	0	-4.626957	0.019853	-0.337702
18	6	0	-4.011358	0.016234	0.874417
19	6	0	-2.543685	0.006142	0.895868
20	7	0	-1.909726	-0.001857	-0.352234
21	6	0	-2.521067	0.001248	-1.598435

22	6	0	-4.755234	0.022802	2.183025
23	8	0	-1.874206	0.003207	1.945099
24	8	0	-1.918489	-0.006595	-2.668747
25	1	0	-4.406536	0.016533	-2.416187
26	1	0	-0.853079	-0.014356	-0.359512
27	1	0	-5.709491	0.027793	-0.438500
28	1	0	-4.495266	-0.857956	2.784034
29	1	0	-4.483279	0.901241	2.782096
30	1	0	-5.839101	0.029902	2.020118

mA...mT H
-1000.190056752866

1	7	0	1.430497	-2.589894	-0.014706
2	6	0	2.430757	-1.681537	-0.005430
3	7	0	3.717025	-2.122178	0.000194
4	6	0	4.715770	-1.219024	0.008076
5	7	0	4.640566	0.126663	0.011390
6	6	0	3.359845	0.534987	0.005919
7	6	0	2.214880	-0.278124	-0.002497
8	7	0	1.068892	0.507817	-0.005751
9	6	0	1.508301	1.756855	0.000306
10	7	0	2.885492	1.842503	0.007740
11	1	0	5.722376	-1.637553	0.011971
12	1	0	0.867495	2.630942	0.000070
13	6	0	3.703173	3.055374	0.013969
14	1	0	1.687760	-3.568267	-0.010509
15	1	0	0.438873	-2.332530	-0.011094
16	1	0	4.346167	3.070491	0.900237
17	1	0	4.336345	3.087559	-0.879016
18	1	0	3.040816	3.925242	0.025897
19	7	0	-1.716857	0.088080	-0.008749
20	6	0	-2.421320	1.280075	-0.005009
21	7	0	-3.822784	1.129769	-0.001246
22	6	0	-4.406320	-0.123870	0.005910
23	6	0	-3.701958	-1.289045	0.005428
24	6	0	-2.241805	-1.207017	-0.002503
25	8	0	-1.885610	2.390656	-0.004356
26	8	0	-1.488655	-2.197765	-0.003889
27	6	0	-4.354443	-2.646158	0.012375
28	6	0	-4.626646	2.364452	0.006922
29	1	0	-0.667322	0.187901	-0.011061
30	1	0	-5.493750	-0.126930	0.011281
31	1	0	-4.051818	-3.228806	-0.867078
32	1	0	-5.447073	-2.559737	0.017547
33	1	0	-4.043141	-3.224012	0.891965
34	1	0	-4.395062	2.972272	-0.873692
35	1	0	-4.403500	2.956270	0.900724
36	1	0	-5.685769	2.095791	-0.000683

8oG...C WC pl
-1012.943554208613

1	7	0	-0.797630	-0.001184	-4.275321
2	6	0	-0.814669	0.000195	-2.892456
3	6	0	0.516760	-0.001064	-2.473178
4	7	0	1.321067	-0.002902	-3.621965
5	6	0	0.534328	-0.002726	-4.773823
6	6	0	0.825277	0.000509	-1.096550
7	7	0	-0.352142	0.002418	-0.305606
8	6	0	-1.636693	0.003900	-0.803293
9	7	0	-1.913149	0.002583	-2.113545
10	8	0	1.964777	0.000429	-0.559730
11	7	0	-2.652562	0.008771	0.095378
12	8	0	0.884980	-0.004370	-5.947601
13	1	0	-1.607386	-0.000732	-4.881020
14	1	0	-0.206502	0.001609	0.725020
15	1	0	-3.592382	0.003332	-0.273319
16	1	0	-2.496899	0.001521	1.109432
17	1	0	2.330777	-0.004090	-3.642668
18	7	0	2.392767	0.005233	2.201346
19	6	0	1.370501	0.002824	3.073446
20	6	0	1.616137	0.002866	4.497717
21	6	0	0.530181	-0.000390	5.318182
22	7	0	-0.729982	-0.003518	4.791852
23	6	0	-0.971677	-0.003292	3.389205
24	7	0	0.119876	0.000483	2.571338
25	8	0	-2.148710	-0.006612	2.991446
26	1	0	-1.550700	-0.006190	5.387337
27	1	0	0.606389	-0.000767	6.401501
28	1	0	2.622026	0.005305	4.902195
29	1	0	3.342900	0.006067	2.545479
30	1	0	2.224514	0.003777	1.170980

I...C WC pl
-882.2753519981751

1	6	0	-0.075129	0.000000	0.004788
2	7	0	-0.032964	0.000000	1.435994
3	6	0	1.136321	0.000000	2.138849
4	6	0	2.333113	0.000000	1.487836
5	6	0	2.296576	0.000000	0.043627
6	7	0	1.137551	0.000000	-0.634966
7	8	0	-1.167239	0.000000	-0.567902
8	7	0	3.436575	0.000000	-0.675054
9	1	0	-0.930872	0.000000	1.907121
10	1	0	1.055015	0.000000	3.222163
11	1	0	3.268450	0.000000	2.036016
12	1	0	4.330777	0.000000	-0.205491
13	1	0	3.404023	0.000000	-1.711972

14	8	0	3.286839	0.000000	-3.523239
15	6	0	2.215829	0.000000	-4.158525
16	7	0	0.968727	0.000000	-3.479609
17	6	0	-0.261782	0.000000	-4.068414
18	7	0	-0.475079	0.000000	-5.370296
19	6	0	0.690305	0.000000	-6.071351
20	6	0	2.010875	0.000000	-5.585686
21	7	0	2.922186	0.000000	-6.631917
22	6	0	2.178084	0.000000	-7.720164
23	7	0	0.817565	0.000000	-7.445314
24	1	0	-1.101773	0.000000	-3.375619
25	1	0	1.012874	0.000000	-2.431253
26	1	0	2.549762	0.000000	-8.737699
27	1	0	0.052355	0.000000	-8.108553

G...U wobble
-957.5472726989199

1	8	0	-1.334025	-0.032396	0.223481
2	6	0	-0.572489	-0.030876	1.205512
3	7	0	0.838675	-0.051278	1.001679
4	6	0	1.795664	-0.040326	1.987903
5	7	0	1.520125	-0.005698	3.283622
6	6	0	0.184198	0.002574	3.524198
7	6	0	-0.883354	-0.007719	2.607562
8	7	0	-2.105415	0.014935	3.269145
9	6	0	-1.792312	0.037427	4.545870
10	7	0	-0.415510	0.032267	4.764433
11	7	0	3.109277	-0.122878	1.573422
12	1	0	1.140016	-0.065245	0.012178
13	1	0	-2.494636	0.058046	5.370176
14	1	0	0.068237	0.043121	5.653651
15	1	0	3.790078	0.128326	2.280150
16	1	0	3.327481	0.170588	0.627760
17	8	0	1.730602	0.021840	-1.684278
18	6	0	0.910717	0.015292	-2.621894
19	7	0	-0.453465	-0.012438	-2.473806
20	6	0	-1.421512	-0.022787	-3.530402
21	6	0	-0.836682	-0.001655	-4.873524
22	6	0	0.505997	0.026211	-5.033255
23	7	0	1.358268	0.035794	-3.944560
24	8	0	-2.618886	-0.047007	-3.277917
25	1	0	-1.508236	-0.008704	-5.723098
26	1	0	-0.820248	-0.022970	-1.492922
27	1	0	0.989691	0.042658	-6.005409
28	1	0	2.363414	0.051502	-4.066398

CCH+
-790.422242922873

1	6	0	-0.072836	-0.000057	-0.014867
2	7	0	-0.033056	-0.000044	1.390565
3	6	0	1.140385	0.000006	2.089959
4	6	0	2.330005	0.000040	1.428045
5	6	0	2.288826	0.000023	-0.009485
6	7	0	1.116744	-0.000024	-0.687125
7	8	0	-1.188269	-0.000095	-0.578675
8	7	0	3.427264	0.000063	-0.724616
9	1	0	-0.929601	-0.000072	1.867501
10	1	0	1.062512	0.000016	3.172485
11	1	0	3.269301	0.000089	1.968693
12	1	0	4.323629	0.000090	-0.257046
13	1	0	3.403637	0.000027	-1.747956
14	7	0	0.834734	-0.000014	-3.491011
15	6	0	-0.412571	0.000018	-4.062691
16	6	0	-0.498560	0.000023	-5.493833
17	6	0	0.657661	-0.000008	-6.213687
18	7	0	1.878209	-0.000049	-5.594533
19	6	0	2.032840	-0.000044	-4.201595
20	8	0	3.136309	-0.000072	-3.666203
21	7	0	-1.473867	0.000037	-3.269304
22	1	0	2.739525	-0.000075	-6.133742
23	1	0	0.670394	-0.000002	-7.299052
24	1	0	-1.462822	0.000063	-5.987121
25	1	0	-2.397755	0.000045	-3.685461
26	1	0	-1.383581	0.000004	-2.216824
27	1	0	0.942535	-0.000018	-2.423637

U...U Calcutta pl
-829.7966091238592

1	8	0	3.645554	0.317211	-0.004970
2	6	0	3.134715	-0.794703	-0.002725
3	7	0	3.914700	-1.971638	-0.000403
4	6	0	3.382348	-3.240434	0.002916
5	6	0	2.042323	-3.447105	0.003564
6	6	0	1.129105	-2.308010	0.000540
7	7	0	1.764945	-1.044063	-0.002782
8	8	0	-0.103819	-2.395856	0.000474
9	1	0	1.621429	-4.444579	0.006065
10	1	0	4.916614	-1.822778	-0.000548
11	1	0	1.155053	-0.206731	-0.002773
12	1	0	4.103527	-4.052943	0.004937
13	8	0	0.080500	1.324864	-0.002052
14	6	0	-1.157010	1.361027	-0.001587
15	7	0	-1.810289	2.617434	0.001708
16	6	0	-3.184158	2.866383	0.003909
17	7	0	-3.944371	1.686406	0.001125
18	6	0	-3.393431	0.420390	-0.002798
19	6	0	-2.052763	0.216314	-0.004293

20	8	0	-3.683305	3.983652	0.007452
21	1	0	-1.615670	-0.777385	-0.008496
22	1	0	-4.948906	1.819052	0.002341
23	1	0	-1.212706	3.440935	0.003579
24	1	0	-4.107965	-0.397528	-0.004941

U...U pl

-829.8011027016166

1	8	0	3.049540	0.007111	-2.392101
2	6	0	3.040621	0.004197	-1.169059
3	7	0	4.231769	0.000570	-0.411873
4	6	0	4.262004	-0.002426	0.963294
5	6	0	3.121890	-0.002375	1.698560
6	6	0	1.830331	0.000630	1.025933
7	7	0	1.892074	0.002920	-0.381160
8	8	0	0.737206	0.001154	1.613334
9	1	0	3.141681	-0.004550	2.780894
10	1	0	5.086905	0.000273	-0.955181
11	1	0	0.986594	0.006115	-0.885594
12	1	0	5.251049	-0.004662	1.412482
13	8	0	-0.714670	-0.004963	-1.591537
14	6	0	-1.777079	-0.003013	-0.954851
15	7	0	-3.008308	-0.003601	-1.620127
16	6	0	-4.223290	-0.001075	-0.963621
17	6	0	-4.296164	0.001884	0.388238
18	6	0	-3.073205	0.002151	1.193244
19	7	0	-1.872684	-0.000113	0.419009
20	8	0	-3.025127	0.004363	2.418501
21	1	0	-5.248463	0.003800	0.903785
22	1	0	-2.957034	-0.005335	-2.631759
23	1	0	-0.969634	-0.001102	0.930895
24	1	0	-5.100285	-0.001653	-1.604257

6tG...C WC pl

NOT STUDIED

A...4tU WC

NOT STUDIED

2-aminoA...T

-976.9761531785853

1	7	0	-0.930954	0.287711	-2.007775
2	6	0	-1.610940	0.102305	-0.848969
3	7	0	-0.922757	-0.065767	0.307777
4	6	0	-1.616662	-0.226271	1.478707
5	7	0	-2.960931	-0.231625	1.637819
6	6	0	-3.600861	-0.068689	0.472090
7	6	0	-3.026235	0.103723	-0.796545

8	7	0	-4.001843	0.237952	-1.783617
9	6	0	-5.140665	0.150713	-1.128514
10	7	0	-4.965599	-0.033648	0.242636
11	7	0	-0.862360	-0.444015	2.604357
12	1	0	-6.128942	0.211500	-1.567594
13	1	0	-5.687357	-0.132497	0.944738
14	1	0	0.068224	0.065446	-2.056183
15	1	0	-1.468981	0.284494	-2.864671
16	1	0	-1.367683	-0.361056	3.477376
17	1	0	0.110444	-0.133368	2.607530
18	8	0	1.933857	-0.307337	-2.019760
19	6	0	2.602578	-0.139296	-0.988014
20	7	0	1.968293	0.020999	0.256506
21	6	0	2.596169	0.228380	1.471304
22	7	0	3.991031	0.267124	1.390321
23	6	0	4.692479	0.110746	0.210600
24	6	0	4.070018	-0.092054	-0.979258
25	8	0	2.009434	0.369934	2.548675
26	6	0	4.804024	-0.263330	-2.281878
27	1	0	4.474395	0.415960	2.268141
28	1	0	0.908794	-0.018635	0.275417
29	1	0	5.774261	0.162786	0.302341
30	1	0	4.560032	-1.229153	-2.741927
31	1	0	4.505614	0.509749	-3.001151
32	1	0	5.888312	-0.207295	-2.133390

2-aminoA...T pl
-976.9757844528147

1	7	0	0.390842	5.319442	0.000000
2	6	0	-0.993556	5.491504	0.000000
3	7	0	-1.650939	4.350714	0.000000
4	6	0	-0.651886	3.377857	0.000000
5	6	0	0.626230	3.954787	0.000000
6	7	0	1.804111	3.317660	0.000000
7	6	0	1.648276	1.970876	0.000000
8	7	0	0.466570	1.270607	0.000000
9	6	0	-0.701871	1.961353	0.000000
10	7	0	2.790915	1.229847	0.000000
11	7	0	-1.876287	1.291487	0.000000
12	1	0	1.098161	6.042745	0.000000
13	1	0	-1.439363	6.478601	0.000000
14	1	0	-1.912334	0.268844	0.000000
15	1	0	-2.732456	1.828183	0.000000
16	1	0	3.669215	1.726208	0.000000
17	1	0	2.776561	0.211486	0.000000
18	6	0	1.633337	-2.294818	0.000000
19	7	0	0.405690	-1.655964	0.000000
20	6	0	-0.852778	-2.285601	0.000000
21	6	0	-0.845793	-3.753871	0.000000

22	6	0	0.356398	-4.384687	0.000000
23	7	0	1.549867	-3.689379	0.000000
24	6	0	-2.164372	-4.479298	0.000000
25	8	0	-1.895924	-1.614651	0.000000
26	8	0	2.725336	-1.718475	0.000000
27	1	0	0.425996	-0.597013	0.000000
28	1	0	2.437525	-4.177672	0.000000
29	1	0	0.448655	-5.467629	0.000000
30	1	0	-2.759930	-4.204042	-0.879482
31	1	0	-2.016266	-5.565058	0.000000
32	1	0	-2.759930	-4.204042	0.879482

A...F

-937.4723652269310

1	7	0	-5.252765	0.523877	0.042431
2	6	0	-5.451313	-0.849758	0.033799
3	1	0	-6.447098	-1.276186	0.050635
4	7	0	-4.325407	-1.537074	0.004851
5	6	0	-3.331431	-0.561792	-0.007527
6	6	0	-1.917378	-0.636898	-0.036567
7	7	0	-1.245051	-1.815253	-0.072368
8	1	0	-1.756408	-2.685101	-0.025838
9	1	0	-0.232605	-1.821104	-0.045736
10	7	0	-1.213625	0.521394	-0.036931
11	6	0	-1.885597	1.692176	-0.012502
12	1	0	-1.262531	2.586279	-0.013947
13	7	0	-3.214279	1.897092	0.014291
14	6	0	-3.883461	0.731086	0.015909
15	1	0	-5.961628	1.246172	0.063875
16	6	0	4.418350	1.404780	0.006746
17	6	0	4.951512	0.110547	0.018673
18	1	0	6.032015	-0.016284	0.030184
19	6	0	4.136554	-1.033532	0.016291
20	6	0	4.697242	-2.437470	0.029037
21	1	0	4.355088	-2.995695	0.910162
22	1	0	4.373599	-3.004292	-0.853595
23	1	0	5.792080	-2.414538	0.040416
24	6	0	2.756996	-0.798980	0.001205
25	9	0	1.918243	-1.904168	-0.001513
26	6	0	2.165307	0.458504	-0.011217
27	1	0	1.081061	0.580650	-0.021938
28	6	0	3.033548	1.548548	-0.007871
29	9	0	2.495240	2.808657	-0.019292
30	1	0	5.059508	2.281159	0.008805

G...4tU

NOT STUDIED

G...2tU

NOTSTUDIED

A...C pl

-862.3789834612737

1	6	0	-1.261750	0.008186	3.321644
2	7	0	-0.842435	0.008961	4.695661
3	6	0	0.468247	0.002046	5.068634
4	6	0	1.450508	-0.005221	4.124619
5	6	0	1.032255	-0.004938	2.740857
6	7	0	-0.259572	0.001236	2.382985
7	8	0	-2.465737	0.013336	3.065983
8	7	0	1.953669	-0.011301	1.752873
9	1	0	-1.586797	0.014059	5.384079
10	1	0	0.674834	0.002793	6.135385
11	1	0	2.497541	-0.010524	4.406336
12	1	0	2.936506	-0.015913	1.985171
13	1	0	1.660502	-0.006654	0.755047
14	7	0	-1.157400	-0.011464	-0.421051
15	6	0	-0.234426	-0.004207	-1.397168
16	7	0	1.092917	0.002480	-1.070011
17	6	0	2.014425	0.010409	-2.057879
18	7	0	1.827007	0.012521	-3.385764
19	6	0	0.512747	0.005250	-3.684787
20	6	0	-0.560968	-0.003243	-2.781006
21	7	0	-1.781994	-0.008811	-3.448247
22	6	0	-1.453907	-0.003831	-4.725937
23	7	0	-0.081400	0.004727	-4.935225
24	1	0	3.052495	0.015704	-1.723229
25	1	0	-2.151922	-0.005995	-5.554355
26	1	0	0.404596	0.009747	-5.823053
27	1	0	-0.885617	-0.007301	0.577034
28	1	0	-2.137115	-0.014940	-0.671906

G...G pl

-1085.292599711964

1	8	0	1.809652	2.381182	0.001779
2	6	0	0.605995	2.665907	-0.015084
3	7	0	-0.368077	1.620187	-0.134857
4	6	0	-1.732955	1.775171	-0.171937
5	7	0	-2.339585	2.956696	-0.084557
6	6	0	-1.455967	3.979163	0.029672
7	6	0	-0.050183	3.946416	0.070241
8	7	0	0.472557	5.229808	0.195305
9	6	0	-0.579810	6.017901	0.231637
10	7	0	-1.780561	5.316787	0.136255
11	7	0	-2.487703	0.643532	-0.351780
12	1	0	0.033029	0.666500	-0.176400
13	1	0	-0.561620	7.097016	0.324779

14	1	0	-2.718857	5.696012	0.136456
15	1	0	-3.479814	0.758848	-0.190653
16	1	0	-2.104513	-0.285274	-0.177651
17	8	0	-1.814179	-2.397282	-0.033904
18	6	0	-0.687786	-2.902700	-0.024430
19	7	0	-0.539813	-4.333852	0.039372
20	6	0	0.658808	-5.023829	0.065534
21	7	0	1.841041	-4.435341	0.036094
22	6	0	1.755293	-3.081783	-0.043133
23	6	0	0.603739	-2.284820	-0.072733
24	7	0	0.940956	-0.945737	-0.141290
25	6	0	2.258127	-0.911383	-0.149709
26	7	0	2.804970	-2.186900	-0.093643
27	7	0	0.585820	-6.404928	0.063350
28	1	0	-1.417471	-4.846839	0.011291
29	1	0	2.846370	-0.001779	-0.186188
30	1	0	3.789148	-2.425536	-0.086602
31	1	0	1.476415	-6.852523	0.253800
32	1	0	-0.199944	-6.835323	0.538989

G...6tG pl
NOT STUDIED

6tG...G pl
NOT STUDIED

G...A 1
-1010.026376044906

1	8	0	-1.331373	0.264843	-1.917627
2	6	0	-2.028266	0.131623	-0.897847
3	7	0	-1.402621	-0.000676	0.377682
4	6	0	-2.057140	-0.200222	1.568553
5	7	0	-3.374201	-0.264995	1.693604
6	6	0	-4.010961	-0.101696	0.505920
7	6	0	-3.459537	0.083439	-0.773666
8	7	0	-4.459224	0.184934	-1.734279
9	6	0	-5.582076	0.067352	-1.059778
10	7	0	-5.374688	-0.110092	0.306907
11	7	0	-1.264533	-0.287145	2.701434
12	1	0	-0.362259	0.098114	0.391563
13	1	0	-6.579966	0.099711	-1.479738
14	1	0	-6.076124	-0.225341	1.027697
15	1	0	-1.759113	-0.641732	3.512732
16	1	0	-0.333178	-0.669830	2.578252
17	7	0	1.482619	-0.249790	-1.841117
18	6	0	2.178090	-0.052103	-0.705901
19	7	0	1.509985	0.202631	0.458657
20	6	0	2.216869	0.416561	1.591938
21	7	0	3.544459	0.398611	1.769658

22	6	0	4.182130	0.128947	0.613089
23	6	0	3.596163	-0.102651	-0.641509
24	7	0	4.562475	-0.333909	-1.614643
25	6	0	5.706183	-0.247198	-0.962989
26	7	0	5.543653	0.030645	0.387516
27	1	0	1.619111	0.643051	2.475974
28	1	0	6.689541	-0.373042	-1.399539
29	1	0	6.270779	0.149797	1.081702
30	1	0	0.465980	-0.066908	-1.884632
31	1	0	2.000075	-0.375350	-2.701448

G...A 1 p
-1010.026368718737

1	7	0	0.462865	-1.505828	0.199336
2	6	0	1.597576	-2.202428	0.437905
3	7	0	1.781550	-3.529239	0.449967
4	6	0	0.630296	-4.178006	0.183942
5	6	0	-0.624997	-3.603194	-0.070764
6	6	0	-0.696467	-2.184738	-0.050949
7	7	0	0.411896	-5.542381	0.112610
8	6	0	-0.935430	-5.717358	-0.172638
9	7	0	-1.591613	-4.578865	-0.289734
10	1	0	1.108476	-6.263438	0.252888
11	1	0	-1.366375	-6.705245	-0.281128
12	1	0	2.476570	-1.595635	0.659652
13	7	0	-1.832811	-1.498624	-0.273095
14	1	0	-2.690046	-2.022491	-0.393215
15	1	0	-1.881458	-0.478562	-0.111269
16	6	0	1.571312	2.066753	-0.145203
17	7	0	0.377766	1.403535	0.002056
18	6	0	-0.902523	2.022217	0.121864
19	6	0	-0.781513	3.454462	0.120429
20	6	0	0.500799	4.014227	-0.014785
21	7	0	1.694197	3.385535	-0.166207
22	7	0	0.297888	5.377086	0.013661
23	6	0	-1.073424	5.575875	0.162544
24	7	0	-1.747422	4.448389	0.227595
25	7	0	2.708854	1.280177	-0.226676
26	1	0	2.599210	0.360656	-0.640728
27	1	0	3.527540	1.787394	-0.544562
28	1	0	0.392768	0.360443	0.073691
29	8	0	-1.923578	1.319731	0.208971
30	1	0	-1.497151	6.571319	0.214756
31	1	0	1.019339	6.083344	-0.060908

G...A 2
-1010.017306766861

1	8	0	-1.333600	-0.276912	-5.291151
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2	6	0	-1.268619	-0.171683	-4.072482
3	7	0	0.003616	-0.414844	-3.406767
4	6	0	0.259286	-0.354652	-2.052908
5	7	0	-0.684841	-0.044166	-1.168258
6	6	0	-1.893702	0.211261	-1.736755
7	6	0	-2.264342	0.175405	-3.089464
8	7	0	-3.604792	0.508545	-3.244060
9	6	0	-4.035591	0.741838	-2.024609
10	7	0	-3.040298	0.571798	-1.061647
11	7	0	1.513233	-0.665167	-1.608785
12	1	0	0.746900	-0.676961	-4.048910
13	1	0	-5.042044	1.033172	-1.750685
14	1	0	-3.115360	0.735232	-0.065255
15	1	0	1.753837	-0.357341	-0.650760
16	1	0	2.272062	-0.666904	-2.278317
17	7	0	-0.630700	-0.835645	1.712677
18	6	0	0.288732	-0.499204	2.647222
19	7	0	-0.031217	-0.654320	3.957693
20	6	0	0.872946	-0.315797	4.896255
21	7	0	2.112214	0.185436	4.730642
22	6	0	2.406484	0.313736	3.427767
23	6	0	1.583332	-0.004184	2.333034
24	7	0	2.251045	0.239984	1.131930
25	6	0	3.436480	0.700246	1.493000
26	7	0	3.588388	0.771164	2.863067
27	1	0	0.554391	-0.464724	5.927796
28	1	0	4.227452	0.996637	0.815335
29	1	0	4.404752	1.084612	3.373033
30	1	0	-1.521034	-1.177828	2.051998
31	1	0	-0.530022	-0.583745	0.720621

G...A 2 pl
-1010.015762617445

1	6	0	1.288204	1.648969	0.000580
2	7	0	-0.022362	1.407189	0.000481
3	6	0	-0.776483	2.540161	-0.000044
4	6	0	-0.366420	3.882723	-0.000432
5	6	0	1.043836	4.177451	-0.000390
6	7	0	1.796434	2.933349	-0.000030
7	7	0	2.165798	0.613620	0.001379
8	7	0	-1.462247	4.737408	-0.001110
9	6	0	-2.507906	3.942603	-0.001025
10	7	0	-2.154860	2.592419	-0.000262
11	1	0	-2.783786	1.800076	-0.000637
12	1	0	-3.545078	4.254303	-0.001366
13	8	0	1.650714	5.241982	-0.000979
14	1	0	2.802621	3.077513	-0.000004
15	1	0	1.831452	-0.363652	0.001012
16	1	0	3.160070	0.785524	0.000173

17	6	0	2.312744	-3.197459	-0.000448
18	7	0	1.400678	-2.240202	-0.000026
19	6	0	0.178359	-2.912864	0.000289
20	7	0	1.760600	-4.461864	-0.000625
21	6	0	0.382192	-4.304358	-0.000203
22	6	0	-1.174917	-2.479943	0.000898
23	7	0	-2.145432	-3.430362	-0.000124
24	6	0	-1.790792	-4.728787	-0.000832
25	7	0	-0.554864	-5.264471	-0.000719
26	1	0	3.384600	-3.043293	-0.001112
27	1	0	2.254462	-5.345525	-0.001232
28	1	0	-2.617068	-5.439394	-0.001864
29	7	0	-1.552688	-1.181746	0.002479
30	1	0	-0.897413	-0.389479	0.004123
31	1	0	-2.549653	-1.007495	0.002053

G...A 3
-1010.024863356307

1	8	0	1.052447	-1.817824	-0.388597
2	6	0	1.802678	-0.850742	-0.187707
3	7	0	1.243458	0.438206	0.062445
4	6	0	1.956829	1.577343	0.340647
5	7	0	3.277977	1.636965	0.386688
6	6	0	3.854844	0.437363	0.114612
7	6	0	3.239776	-0.796164	-0.160719
8	7	0	4.190398	-1.789893	-0.360361
9	6	0	5.346230	-1.179506	-0.213603
10	7	0	5.207374	0.176023	0.077456
11	7	0	1.215575	2.736726	0.534310
12	1	0	0.208960	0.516815	-0.033535
13	1	0	6.322173	-1.641038	-0.301166
14	1	0	5.944475	0.851644	0.235960
15	1	0	1.759830	3.485317	0.950715
16	1	0	0.300326	2.610682	0.955744
17	7	0	-1.688378	-2.183394	0.419079
18	6	0	-2.761578	-1.380150	0.260082
19	7	0	-4.003298	-1.917370	0.402597
20	6	0	-5.082462	-1.133289	0.234457
21	7	0	-5.135282	0.176868	-0.081261
22	6	0	-3.900306	0.686003	-0.201029
23	6	0	-2.678971	0.010565	-0.034032
24	7	0	-1.611013	0.888234	-0.223849
25	6	0	-2.169674	2.053202	-0.510778
26	7	0	-3.546802	1.993132	-0.511164
27	1	0	-6.044888	-1.628184	0.364351
28	1	0	-1.629346	2.965322	-0.733007
29	1	0	-4.192099	2.748475	-0.705484
30	1	0	-1.882281	-3.170673	0.539713
31	1	0	-0.740124	-1.919202	0.118002

G...A 4

-1010.018266198239

1	8	0	5.426196	-1.583334	0.061741
2	6	0	4.362877	-0.974880	0.046954
3	7	0	3.118990	-1.716772	0.179306
4	6	0	1.837699	-1.203892	0.195705
5	7	0	1.598928	0.101945	0.076901
6	6	0	2.729505	0.846066	-0.061540
7	6	0	4.069610	0.429934	-0.086740
8	7	0	4.922989	1.514376	-0.250955
9	6	0	4.128754	2.558295	-0.325069
10	7	0	2.780833	2.215778	-0.212925
11	7	0	0.798461	-2.067177	0.381293
12	1	0	3.260807	-2.716470	0.297489
13	1	0	4.440399	3.587140	-0.456472
14	1	0	1.986005	2.839819	-0.267311
15	1	0	-0.159452	-1.726709	0.171414
16	1	0	0.962166	-3.054906	0.235228
17	7	0	-1.224785	1.052393	0.424471
18	6	0	-2.232464	0.199773	0.140073
19	7	0	-1.946599	-1.100622	-0.145527
20	6	0	-2.960802	-1.949485	-0.428249
21	7	0	-4.276892	-1.698278	-0.471033
22	6	0	-4.533503	-0.408761	-0.180416
23	6	0	-3.596169	0.589583	0.130488
24	7	0	-4.218575	1.810412	0.371146
25	6	0	-5.503217	1.555177	0.210794
26	7	0	-5.758694	0.232532	-0.123556
27	1	0	-2.661253	-2.973966	-0.649442
28	1	0	-6.305229	2.275153	0.319610
29	1	0	-6.660665	-0.193516	-0.296256
30	1	0	-0.241114	0.757119	0.337781
31	1	0	-1.455722	2.015168	0.629318

A...A 1 pl

-934.7549758304071

1	7	0	-1.279090	-0.000740	-1.387419
2	6	0	-2.138940	-0.000927	-0.349869
3	7	0	-1.654644	-0.002887	0.924496
4	6	0	-2.524367	-0.003249	1.958785
5	7	0	-3.865480	-0.001855	1.929439
6	6	0	-4.319656	0.000167	0.661420
7	6	0	-3.549752	0.000782	-0.512389
8	7	0	-4.357127	0.003011	-1.646011
9	6	0	-5.586755	0.003708	-1.167968
10	7	0	-5.631735	0.002051	0.219465
11	1	0	-2.068050	-0.004919	2.948932

12	1	0	-6.492483	0.005384	-1.762241
13	1	0	-6.455853	0.002185	0.807149
14	1	0	-0.254610	-0.002056	-1.240703
15	1	0	-1.658782	0.001076	-2.324603
16	7	0	1.278972	-0.000745	1.387340
17	6	0	2.138860	-0.000928	0.349821
18	7	0	1.654630	-0.002884	-0.924573
19	6	0	2.524416	-0.003243	-1.958810
20	7	0	3.865528	-0.001849	-1.929392
21	6	0	4.319635	0.000170	-0.661346
22	6	0	3.549665	0.000781	0.512415
23	7	0	4.356974	0.003007	1.646084
24	6	0	5.586631	0.003707	1.168112
25	7	0	5.631690	0.002054	-0.219317
26	1	0	2.068158	-0.004910	-2.948984
27	1	0	6.492325	0.005381	1.762438
28	1	0	6.455843	0.002190	-0.806955
29	1	0	0.254487	-0.002060	1.240600
30	1	0	1.658650	0.001069	2.324531

A...A 2 pl
-934.7534750390968

1	7	0	-1.131657	0.003186	-1.475832
2	6	0	-1.956430	0.002554	-0.409444
3	7	0	-1.430394	-0.001774	0.846289
4	6	0	-2.267480	-0.002633	1.907481
5	7	0	-3.608816	0.000368	1.921916
6	6	0	-4.103771	0.004762	0.669584
7	6	0	-3.371321	0.006143	-0.528026
8	7	0	-4.213972	0.010960	-1.635750
9	6	0	-5.428030	0.012360	-1.118744
10	7	0	-5.429131	0.008853	0.269185
11	1	0	-1.779946	-0.006210	2.882751
12	1	0	-6.351964	0.015897	-1.684280
13	1	0	-6.234481	0.009124	0.882430
14	1	0	-0.106180	0.000403	-1.365764
15	1	0	-1.542761	0.007040	-2.399530
16	7	0	1.841982	-0.001566	-1.293845
17	6	0	2.742763	-0.002571	-0.227882
18	6	0	2.583806	-0.002301	1.185857
19	7	0	3.710702	-0.003307	1.948315
20	6	0	4.911827	-0.004594	1.343228
21	7	0	5.194086	-0.005050	0.025397
22	6	0	4.066479	-0.003986	-0.702612
23	7	0	3.948973	-0.003972	-2.085138
24	6	0	2.599666	-0.002409	-2.376736
25	7	0	1.388303	-0.001224	1.811280
26	1	0	5.772345	-0.005304	2.012426
27	1	0	2.236167	-0.001996	-3.396855

28	1	0	4.717984	-0.004756	-2.743181
29	1	0	1.405890	-0.000982	2.823372
30	1	0	0.479234	-0.001181	1.325211

A...A 3 pl
-934.7516934249100

1	7	0	1.776044	-0.737439	1.263368
2	6	0	1.151620	-0.431327	2.425745
3	7	0	1.840928	-0.555577	3.589253
4	6	0	1.225216	-0.254243	4.748525
5	7	0	-0.033466	0.182761	4.946637
6	6	0	-0.693657	0.283400	3.782052
7	6	0	-0.201941	-0.006449	2.497170
8	7	0	-1.190600	0.196844	1.535083
9	6	0	-2.244539	0.607053	2.218678
10	7	0	-2.006290	0.683297	3.577446
11	1	0	1.832503	-0.375824	5.645460
12	1	0	-3.207033	0.862320	1.792713
13	1	0	-2.658138	0.965069	4.298686
14	1	0	2.764809	-0.946987	1.331502
15	1	0	1.408857	-0.428960	0.354088
16	7	0	-1.773661	-0.744036	-1.262259
17	6	0	-1.150453	-0.436602	-2.424865
18	7	0	-1.840729	-0.560781	-3.587801
19	6	0	-1.226528	-0.257703	-4.747407
20	7	0	0.031508	0.180768	-4.946391
21	6	0	0.692662	0.281408	-3.782360
22	6	0	0.202485	-0.009888	-2.497206
23	7	0	1.191821	0.194006	-1.535949
24	6	0	2.244685	0.605801	-2.220269
25	7	0	2.005195	0.682160	-3.578795
26	1	0	-1.834400	-0.379681	-5.643889
27	1	0	3.207336	0.861773	-1.795082
28	1	0	2.656224	0.964540	-4.300537
29	1	0	-2.761875	-0.956251	-1.329623
30	1	0	-1.405693	-0.437404	-0.352797

8oG...G
-1160.572934601169

1	6	0	-5.374553	2.199702	-0.116962
2	7	0	-4.070895	2.341797	-0.023718
3	6	0	-3.575901	1.042859	0.000084
4	7	0	-5.770508	0.863625	-0.158359
5	6	0	-4.621910	0.105372	-0.083044
6	7	0	-2.210205	-0.873419	0.079176
7	6	0	-3.311156	-1.692631	-0.007458
8	7	0	-4.557878	-1.249653	-0.098374
9	7	0	-3.073546	-3.048382	0.056460

10	1	0	-6.098225	3.004513	-0.159628
11	1	0	-2.143889	-3.383333	-0.171467
12	1	0	-3.845522	-3.630618	-0.243849
13	1	0	-6.713165	0.500946	-0.225918
14	1	0	-1.275372	-1.321597	0.122827
15	6	0	-2.228984	0.550804	0.081006
16	8	0	-1.160467	1.185070	0.143577
17	7	0	1.312715	-0.131219	0.050504
18	6	0	1.252938	-1.507085	0.019232
19	7	0	2.589804	-1.942751	-0.032159
20	6	0	3.447354	-0.855980	-0.030716
21	6	0	2.648614	0.281477	0.021690
22	8	0	0.248736	-2.246436	0.034185
23	6	0	3.240167	1.581774	0.026704
24	7	0	4.687935	1.443494	-0.022350
25	6	0	5.387155	0.261669	-0.064326
26	7	0	4.802206	-0.924680	-0.061366
27	8	0	2.729161	2.698512	0.058164
28	7	0	6.767378	0.337837	-0.175584
29	1	0	7.224922	1.114468	0.290666
30	1	0	7.224425	-0.554627	-0.017320
31	1	0	2.858193	-2.917456	-0.060141
32	1	0	0.455600	0.461094	0.093412
33	1	0	5.180070	2.331052	-0.085600

2tU....2tU pl
NOT STUDIED

G...C S
-937.6422515260721

1	8	0	-1.378840	-2.580062	0.703255
2	6	0	-1.154038	-1.395566	0.955018
3	7	0	-0.112039	-1.043271	1.879924
4	6	0	0.351298	0.226036	2.142496
5	7	0	-0.228414	1.320272	1.671700
6	6	0	-1.272577	1.045488	0.849848
7	6	0	-1.765236	-0.199892	0.432185
8	7	0	-2.763127	-0.043409	-0.522836
9	6	0	-2.890683	1.260466	-0.661368
10	7	0	-2.017602	1.974080	0.152687
11	7	0	1.464975	0.320087	2.961070
12	1	0	0.409268	-1.838097	2.241359
13	1	0	-3.589303	1.762276	-1.319543
14	1	0	-1.915735	2.979296	0.215288
15	1	0	1.791593	1.282052	3.008179
16	1	0	2.227282	-0.290188	2.661098
17	6	0	2.317722	-0.005530	-0.503106
18	7	0	2.202499	1.246691	-1.191965
19	6	0	1.246674	1.485211	-2.133784

20	6	0	0.377480	0.497913	-2.487524
21	6	0	0.532145	-0.771613	-1.820999
22	7	0	1.467130	-1.003038	-0.896246
23	8	0	3.150781	-0.097713	0.407946
24	7	0	-0.302270	-1.804094	-2.145854
25	1	0	2.830244	1.981155	-0.884462
26	1	0	1.222066	2.481131	-2.567268
27	1	0	-0.392616	0.665089	-3.231449
28	1	0	-1.209445	-1.555956	-2.526257
29	1	0	-0.339998	-2.558416	-1.462668

mG...mC S
-1016.242057641356

1	8	0	-1.794969	-2.813890	-0.106803
2	6	0	-1.346566	-1.833009	0.485586
3	7	0	-0.168623	-1.964704	1.304129
4	6	0	0.527353	-0.942504	1.906362
5	7	0	0.110078	0.314158	1.910635
6	6	0	-1.046323	0.483971	1.215938
7	6	0	-1.794164	-0.463276	0.499621
8	7	0	-2.845798	0.144840	-0.169702
9	6	0	-2.742786	1.420457	0.147881
10	7	0	-1.673561	1.693562	0.995227
11	7	0	1.704417	-1.292119	2.552155
12	1	0	0.231400	-2.899555	1.311266
13	1	0	-3.405852	2.211239	-0.183819
14	6	0	-1.237166	2.995749	1.492835
15	1	0	2.194024	-0.459576	2.870537
16	1	0	2.324366	-1.852198	1.965415
17	1	0	-0.250306	3.247934	1.087482
18	1	0	-1.962485	3.752183	1.179980
19	1	0	-1.174018	2.983067	2.585899
20	6	0	2.069048	-0.285343	-0.869318
21	7	0	1.990692	1.160040	-0.906325
22	6	0	0.963725	1.780204	-1.552696
23	6	0	-0.008986	1.069567	-2.192051
24	6	0	0.088246	-0.361743	-2.128940
25	7	0	1.095346	-0.988734	-1.520485
26	8	0	2.992554	-0.799579	-0.223167
27	7	0	-0.877518	-1.134604	-2.714746
28	6	0	2.973756	1.914182	-0.116218
29	1	0	0.958186	2.867191	-1.527558
30	1	0	-0.824307	1.571036	-2.700326
31	1	0	-1.794291	-0.713725	-2.821361
32	1	0	-0.904471	-2.099978	-2.395071
33	1	0	3.983577	1.568157	-0.351681
34	1	0	2.791727	1.756440	0.953596
35	1	0	2.882445	2.979180	-0.351342

A...T S

-921.5840124662975

1	7	0	0.287559	2.519129	-0.583894
2	6	0	-1.097430	2.527121	-0.549254
3	1	0	-1.673084	3.098033	-1.267006
4	7	0	-1.600162	1.783708	0.418465
5	6	0	-0.482312	1.243353	1.046729
6	6	0	-0.333167	0.324612	2.112638
7	7	0	-1.400528	-0.212092	2.772819
8	1	0	-1.202017	-1.014813	3.359090
9	1	0	-2.286822	-0.225979	2.279760
10	7	0	0.917175	-0.024886	2.496128
11	6	0	1.965043	0.488209	1.820498
12	1	0	2.946932	0.167385	2.168454
13	7	0	1.960712	1.329870	0.768976
14	6	0	0.706983	1.680534	0.434298
15	1	0	0.870651	2.919185	-1.308304
16	7	0	1.275645	-0.698893	-1.983508
17	6	0	1.402229	-1.622094	-0.961278
18	1	0	2.421206	-1.928341	-0.743417
19	6	0	0.337767	-2.104643	-0.270002
20	6	0	0.466884	-3.093834	0.855680
21	1	0	0.179231	-2.632457	1.807981
22	1	0	-0.193823	-3.954490	0.695287
23	1	0	1.498979	-3.449379	0.948272
24	6	0	-0.997227	-1.601032	-0.612469
25	8	0	-2.043235	-1.901578	-0.035380
26	7	0	-1.024109	-0.687680	-1.699704
27	1	0	-1.929157	-0.271006	-1.903460
28	6	0	0.059356	-0.143783	-2.382138
29	8	0	-0.030464	0.736338	-3.236250
30	1	0	2.099874	-0.303064	-2.419164

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-1000.185758766295

1	7	0	-0.322674	1.829934	1.634419
2	6	0	-1.648463	1.424546	1.643210
3	1	0	-2.450638	2.152997	1.653246
4	7	0	-1.809634	0.112892	1.630267
5	6	0	-0.512584	-0.382138	1.604193
6	6	0	0.011926	-1.694863	1.551516
7	7	0	-0.785077	-2.803331	1.525714
8	1	0	-0.326884	-3.672255	1.275693
9	1	0	-1.731005	-2.683237	1.178896
10	7	0	1.356772	-1.856749	1.542620
11	6	0	2.136215	-0.757705	1.547258
12	1	0	3.209885	-0.945580	1.531328
13	7	0	1.767299	0.537926	1.558985

14	6	0	0.428292	0.665172	1.600716
15	6	0	0.175289	3.205196	1.550939
16	1	0	0.005536	3.600421	0.543797
17	1	0	-0.340806	3.830182	2.286936
18	1	0	1.245516	3.196585	1.773009
19	7	0	0.788465	1.022682	-1.732917
20	6	0	1.243363	-0.283048	-1.806728
21	1	0	2.323697	-0.377007	-1.875772
22	6	0	0.440925	-1.379523	-1.780065
23	6	0	0.973960	-2.784899	-1.835238
24	1	0	0.807607	-3.296379	-0.879437
25	1	0	0.461017	-3.366425	-2.610932
26	1	0	2.050324	-2.789263	-2.038714
27	6	0	-1.000043	-1.175841	-1.638032
28	8	0	-1.846646	-2.065416	-1.520820
29	7	0	-1.390320	0.184882	-1.635650
30	1	0	-2.378725	0.361245	-1.474140
31	6	0	-0.578086	1.313705	-1.614516
32	8	0	-1.025205	2.456670	-1.499344
33	6	0	1.763691	2.124953	-1.646467
34	1	0	2.211042	2.148831	-0.645809
35	1	0	2.546705	1.971823	-2.396160
36	1	0	1.244448	3.063184	-1.845027