The accuracy of quantum chemical methods for large noncovalent complexes

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Table S1
Interaction energies in kcal/mol of the investigated complexes at different DFT-D3 levels of theory. Results for both damping methods "Zero" (Z) and "Becke-Johnson" (BJ) in combination with and without Axilrod-Teller-Mutto "3-body" (3b) correction are presented.

method/complex	CBH	C3A	C3GC	C2C2PD	GCGC	GGG	PHE
ref	-11.06	-18.19	-31.25	-24.36	-14.37	-2.40	-25.76
B3-LYP-D3/QZ(BJ)	-12.96	-17.99	-31.29	-23.22	-15.48	-2.10	-25.99
B3-LYP-D3/QZ(Z)	-13.91	-16.26	-28.25	-19.15	-14.44	-1.76	-26.51
B3-LYP-D3/QZ(BJ+3b)	-12.26	-16.67	-28.87	-21.41	-14.44	-1.82	-25.61
B3-LYP-D3/QZ(Z+3b)	-13.21	-15.04	-25.96	-17.45	-13.44	-1.50	-26.13
B-LYP-D3/QZ(BJ)	-13.42	-18.95	-33.41	-25.59	-16.57	-2.59	-24.96
B-LYP-D3/QZ(Z)	-14.41	-17.81	-31.45	-22.37	-16.38	-2.52	-25.58
B-LYP-D3/QZ(BJ+3b)	-12.73	-18.01	-31.35	-23.79	-15.57	-2.09	-23.92
B-LYP-D3/QZ(Z+3b)	-13.71	-16.57	-29.15	-20.66	-15.38	-2.26	-25.21
TPSS-D3/QZ(BJ)	-12.35	-16.71	-28.58	-21.19	-13.38	-1.87	-24.23
TPSS-D3/QZ(Z)	-13.58	-15.83	-27.19	-18.42	-13.49	-1.93	-24.81
TPSS-D3/QZ(BJ+3b)	-11.65	-15.42	-26.22	-19.43	-12.35	-1.60	-23.86
TPSS-D3/QZ(Z+3b)	-12.88	-14.61	-24.91	-16.72	-12.49	-1.67	-24.44
PW6B95-D3/QZ(BJ)	-10.01	-16.63	-29.71	-19.93	-12.48	-1.70	-24.07
PW6B95-D3/QZ(Z)	-9.74	-14.96	-27.00	-16.28	-11.55	-1.18	-24.35
PW6B95-D3/QZ(BJ+3b)	-9.32	-15.40	-27.42	-18.22	-11.47	-1.44	-23.70
PW6B95-D3/QZ(Z+3b)	-9.05	-13.75	-24.75	-14.60	-10.55	-0.93	-23.99
M06-2X-D3/QZ(BJ)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z)	-8.23	-15.96	-29.00	-20.55	-14.28	-1.71	-25.63
M06-2X-D3/QZ(BJ+3b)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z+3b)	-7.53	-14.77	-26.78	-18.88	-13.29	-1.45	-25.26

Table S2

Signed errors (in kcal/mol) for the investigated complexes at different DFT-D3 level of theory with respect to the reference (QCISD(T)/CBS) data. Negative sign ("-") indicates overestimation of the interaction energy. Results for both damping methods "Zero" (Z) and "Becke-Johnson" (BJ) in combination with and without Axilrod-Teller-Mutto 3-body correction are presented.

method/complex	CBH	C3A	C3GC	C2C2PD	GCGC	GGG	PHE
B3-LYP-D3/QZ(BJ)	-1.90	0.20	-0.03	1.14	-1.12	0.30	-0.23
B3-LYP-D3/QZ(Z)	-2.85	1.93	3.01	5.21	-0.08	0.64	-0.75
B3-LYP-D3/QZ(BJ+3b)	-1.20	1.52	2.38	2.95	-0.07	0.57	0.14
B3-LYP-D3/QZ(Z+3b)	-2.15	3.15	5.30	6.91	0.93	0.90	-0.38
B-LYP-D3/QZ(BJ)	-2.36	-0.76	-2.15	-1.23	-2.21	-0.19	0.80
B-LYP-D3/QZ(Z)	-3.35	0.38	-0.19	1.99	-2.02	-0.12	0.18
B-LYP-D3/QZ(BJ+3b)	-1.67	0.18	-0.09	0.57	-1.20	0.30	1.84
B-LYP-D3/QZ(Z+3b)	-2.66	1.62	2.10	3.70	-1.01	0.14	0.55
TPSS-D3/QZ(BJ)	-1.29	1.48	2.67	3.16	0.99	0.53	1.52
TPSS-D3/QZ(Z)	-2.52	2.36	4.06	5.93	0.88	0.47	0.94
TPSS-D3/QZ(BJ+3b)	-0.59	2.77	5.03	4.93	2.01	0.79	1.90
TPSS-D3/QZ(Z+3b)	-1.82	3.58	6.34	7.63	1.87	0.73	1.32
PW6B95-D3/QZ(BJ)	1.04	1.56	1.55	4.42	1.89	0.70	1.68
PW6B95-D3/QZ(Z)	1.31	3.23	4.26	8.07	2.82	1.22	1.40
PW6B95-D3/QZ(BJ+3b)	1.74	2.79	3.83	6.13	2.90	0.96	2.06
PW6B95-D3/QZ(Z+3b)	2.01	4.44	6.50	9.75	3.82	1.47	1.77
M06-2X-D3/QZ(BJ)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z)	2.83	2.23	2.25	3.81	0.09	0.69	0.13
M06-2X-D3/QZ(BJ+3b)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z+3b)	3.53	3.42	4.48	5.48	1.08	0.95	0.50

Table S3

Relative signed errors (in %) for the investigated complexes at different DFT-D3 level of theory with respect to the reference (QCISD(T)/CBS) data. Negative sign ("-") indicates overestimation of the interaction energy. Results for both damping methods "Zero" (Z) and "Becke-Johnson" (BJ) in combination with and without Axilrod-Teller-Mutto 3-body correction are presented.

method/complex	CBH	C3A	C3GC	C2C2PD	GCGC	GGG	PHE
B3-LYP-D3/QZ(BJ)	-17.19	1.08	-0.11	4.66	-7.78	12.35	-0.91
B3-LYP-D3/QZ(Z)	-25.78	10.59	9.62	21.37	-0.54	26.53	-2.93
B3-LYP-D3/QZ(BJ+3b)	-10.84	8.35	7.62	12.10	-0.50	23.97	0.56
B3-LYP-D3/QZ(Z+3b)	-19.49	17.33	16.94	28.37	6.46	37.42	-1.46
B-LYP-D3/QZ(BJ)	-21.34	-4.20	-6.89	-5.06	-15.35	-8.06	3.09
B-LYP-D3/QZ(Z)	-30.29	2.06	-0.62	8.16	-14.03	-5.14	0.68
B-LYP-D3/QZ(BJ+3b)	-15.11	1.00	-0.30	2.33	-8.35	12.68	7.15
B-LYP-D3/QZ(Z+3b)	-24.01	8.89	6.73	15.19	-7.03	5.73	2.13
TPSS-D3/QZ(BJ)	-11.68	8.14	8.54	12.99	6.86	22.00	5.92
TPSS-D3/QZ(Z)	-22.80	12.98	12.99	24.36	6.09	19.50	3.66
TPSS-D3/QZ(BJ+3b)	-5.33	15.23	16.11	20.24	14.02	33.14	7.37
TPSS-D3/QZ(Z+3b)	-16.48	19.71	20.28	31.33	13.05	30.52	5.12
PW6B95-D3/QZ(BJ)	9.45	8.57	4.95	18.16	13.15	29.06	6.53
PW6B95-D3/QZ(Z)	11.89	17.75	13.62	33.14	19.62	50.75	5.45
PW6B95-D3/QZ(BJ+3b)	15.72	15.35	12.27	25.18	20.15	39.91	8.00
PW6B95-D3/QZ(Z+3b)	18.14	24.39	20.81	40.04	26.56	61.38	6.88
M06-2X-D3/QZ(BJ)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z)	25.59	12.24	7.19	15.64	0.61	28.71	0.50
M06-2X-D3/QZ(BJ+3b)	-	-	-	-	-	-	-
M06-2X-D3/QZ(Z+3b)	31.90	18.39	14.32	22.48	7.50	39.42	1.93

Table S4

The set of statistical measures (in kcal/mol) calculated for the investigated L7 set with respect to the reference (QCISD(T)/CBS) data. Results for both damping methods "Zero" (Z) and "Becke-Johnson" (BJ) in combination with and without Axilrod-Teller-Mutto 3-body correction are presented.

method/stat measure	RMSD	MUE	MSE	MAX
B3-LYP-D3/QZ(BJ)	0.95	0.70	-0.24	1.90
B3-LYP-D3/QZ(Z)	2.64	2.07	1.01	5.21
B3-LYP-D3/QZ(BJ+3b)	1.62	1.26	0.90	2.95
B3-LYP-D3/QZ(Z+3b)	3.63	2.82	2.09	6.91
B-LYP-D3/QZ(BJ)	1.60	1.39	-1.16	2.36
B-LYP-D3/QZ(Z)	1.67	1.17	-0.45	3.35
B-LYP-D3/QZ(BJ+3b)	1.07	0.84	-0.01	1.84
B-LYP-D3/QZ(Z+3b)	2.04	1.68	0.63	3.70
TPSS-D3/QZ(BJ)	1.87	1.66	1.29	3.16
TPSS-D3/QZ(Z)	3.06	2.45	1.73	5.93
TPSS-D3/QZ(BJ+3b)	3.07	2.58	2.41	5.03
TPSS-D3/QZ(Z+3b)	4.15	3.33	2.81	7.63
PW6B95-D3/QZ(BJ)	2.15	1.83	1.83	4.42
PW6B95-D3/QZ(Z)	3.91	3.19	3.19	8.07
PW6B95-D3/QZ(BJ+3b)	3.31	2.92	2.92	6.13
PW6B95-D3/QZ(Z+3b)	5.08	4.25	4.25	9.75
M06-2X-D3/QZ(BJ)	-	-	-	-
M06-2X-D3/QZ(Z)	2.17	1.72	1.72	3.81
M06-2X-D3/QZ(BJ+3b)	-	-	-	-
M06-2X-D3/QZ(Z+3b)	3.30	2.77	2.77	5.48

Table S5
The counterpoise correceted (CPC) and counterpoise uncorrected (noCPC) MP2/CBS binding energies (in kcal/mol) for all seven complexes from L7 set.

complex	CPC	noCPC	difference
CBH	11.80	12.91	1.11
C3A	27.00	31.14	4.14
C3GC	45.12	53.11	7.99
C2C2PD	38.22	42.47	4.25
GCGC	17.85	23.18	5.33
GGG	4.15	6.60	2.46
PHE	25.59	28.04	2.45

Table S5 reveals that there is relatively big difference between counterpoise corrected and uncorrected interaction energies. The absolute (relative) decrease after passing from uncorrected to corrected values range between 1.11 kcal/mol (9 %) for the CBH complex to 5.33 kcal/mol (23 %) for the GCGC complex. Enormously big relative decrease of 37 % (2.46 kcal/mol) in the case of GGG complex can be attributed to relatively small size of the complex, for which the counterpoise correction is more significant, when compared to other clusters.
This points to the fact that presented MP2/CBS values of stabilization energy based on noncounterpoise corrected data are not well converged. We would like to stress at this point that scaled MP2/CBS values presented in manuscript are based on counterpoise corrected data.

Table S6
Binding energies at MP2/DZ, MP2/TZ, MP2-F12/DZ, MP2-F12/TZ, MP2/CBS, scaled MP2/CBS (MP2/CBS`, taken from present work) and MP2-F12/CBS (obtained by Schwenke type extrapolation) levels for GGG and GCGC complexes, are presented, in kcal/mol.

complex	MP2/DZ	MP2-F12/DZ	MP2/TZ	MP2-F12/TZ	MP2/CBS	MP2/CBS`	MP2-F12/CBS	CBS_difference
GGG	0.98	2.61	3.20	3.94	4.15	4.36	4.75	0.39
GCGC	8.67	13.75	15.30	17.53	17.85	18.21	19.78	1.57

Quick inspection of the Table S6 reveals that the relative as well as absolute increase of binding energy when passing from regular to explicitly correlated calculations is significant, especially in the case of DZ basis set (0.98 vs. 2.61 kcal/mol and 8.67 vs. 13.75 kcal/mol for GGG and GCGC, respectively). It is also easy to see that absolute increase of stabilization energy lowers when passing to larger basis set (1.63 and 5.08 kcal/mol at DZ and 0.74 and 2.23 kcal/mol at TZ, for GGG and GCGC, respectively). The relative increase of the stabilization energy at CBS level equals to 14% and 11% for GGG and GCGC complexes, respectively. The same increase, when comparing explicitly correlated MP2/CBS values (MP2-F12/CBS) with respect to scaled MP2/CBS values (MP2/CBS`), equals to 9 % for both complexes. The same quantities in absolute numbers are 0.39 and 1.57 kcal/mol for GGG and GCGC, respectively.
Based on these values we can estimate the relative error in MP2/CBS numbers, presented in manuscript, to be somewhere about 9 %. Because of high computational demands of explicitly correlated calculations we are not able to present these data for remaining complexes in L7 set.

The full xyz geometry information of all seven investigated complexes.

C2C2PD

subsystemA:1-36; subsystemB: 37-72

72

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 -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
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	-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
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

C3A

subsystemA:1-15; subsystemB: 16-87

87

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

C3GC

subsystemA:1-29; subsystemB: 30-101

101

C	-2.997000	2.282000	-1.321000
C	-5.086000	2.109000	-0.090000
C	-4.420000	2.181000	1.091000
C	-2.988000	2.283000	1.033000
C	1.169000	2.375000	1.018000
C	1.174000	2.413000	-1.463000
C	3.126000	2.365000	-0.406000
C	2.588000	2.374000	0.888000
C	4.698000	2.287000	1.157000
N	-4.403000	2.166000	-1.266000
N	-2.330000	2.342000	-0.140000
N	-2.257000	2.321000	2.153000
N	0.537000	2.401000	-0.242000
N	2.498000	2.388000	-1.597000

N	3.587000	2.326000	1.849000
N	4.487000	2.320000	-0.214000
N	0.396000	2.471000	-2.566000
O	-2.454000	2.311000	-2.436000
O	0.482000	2.340000	2.059000
H	-4.871000	2.039000	-2.156000
H	-6.160000	1.987000	-0.158000
H	-4.950000	2.118000	2.032000
H	-2.709000	2.171000	3.044000
H	-1.212000	2.331000	2.112000
H	-0.509000	2.390000	-0.222000
H	5.695000	2.224000	1.569000
H	5.179000	2.214000	-0.945000
H	0.870000	2.330000	-3.447000
H	-0.630000	2.383000	-2.529000
C	6.163000	-0.981000	1.035000
C	5.791000	-0.981000	2.349000
C	4.412000	-0.949000	2.736000
C	3.418000	-0.942000	1.709000
C	3.804000	-0.954000	0.341000
C	5.189000	-0.947000	-0.017000
C	2.814000	-0.909000	-0.675000
C	5.546000	-0.893000	-1.371000
C	4.583000	-0.834000	-2.389000
C	3.196000	-0.853000	-2.040000
C	4.935000	-0.753000	-3.777000
C	3.981000	-0.696000	-4.751000
C	2.583000	-0.728000	-4.433000
C	2.203000	-0.818000	-3.057000
C	0.827000	-0.850000	-2.709000
C	0.443000	-0.917000	-1.339000
C	1.432000	-0.912000	-0.324000
C	2.043000	-0.932000	2.061000
C	1.049000	-0.929000	1.042000
C	-0.325000	-0.947000	1.391000
C	-1.315000	-0.973000	0.377000
C	-0.932000	-0.939000	-0.988000
C	-0.166000	-0.827000	-3.723000
C	-1.543000	-0.881000	-3.373000
C	-1.926000	-0.956000	-2.009000
C	1.588000	-0.684000	-5.418000
C	0.224000	-0.738000	-5.096000
C	-2.546000	-0.865000	-4.392000
C	-3.896000	-0.936000	-4.026000
C	-4.295000	-1.017000	-2.686000
C	-3.301000	-1.010000	-1.657000
C	-2.696000	-1.031000	0.728000
C	-3.685000	-1.075000	-0.289000
C	-0.804000	-0.716000	-6.096000

C	-2.125000	-0.780000	-5.760000
C	-5.069000	-1.143000	0.070000
C	-6.042000	-1.163000	-0.982000
C	-5.673000	-1.095000	-2.297000
C	-5.426000	-1.160000	1.425000
C	-4.466000	-1.086000	2.444000
C	-3.079000	-1.024000	2.095000
C	-2.086000	-0.965000	3.112000
C	-0.711000	-0.919000	2.762000
C	0.281000	-0.885000	3.776000
C	1.658000	-0.887000	3.425000
C	2.660000	-0.869000	4.444000
C	4.012000	-0.908000	4.077000
C	2.238000	-0.816000	5.813000
C	-0.111000	-0.841000	5.151000
C	0.916000	-0.799000	6.151000
C	-2.469000	-0.919000	4.490000
C	-1.475000	-0.850000	5.476000
C	-4.820000	-1.045000	3.833000
C	-3.867000	-0.958000	4.808000
H	7.216000	-0.999000	0.763000
H	6.547000	-0.997000	3.131000
H	6.601000	-0.890000	-1.641000
H	5.989000	-0.737000	-4.041000
H	4.270000	-0.630000	-5.798000
H	1.881000	-0.616000	-6.464000
H	-4.656000	-0.933000	-4.805000
H	-0.507000	-0.650000	-7.140000
H	-2.888000	-0.765000	-6.535000
H	-7.094000	-1.230000	-0.712000
H	-6.430000	-1.112000	-3.078000
H	-6.480000	-1.210000	1.693000
H	4.771000	-0.897000	4.856000
H	3.002000	-0.788000	6.587000
H	0.618000	-0.758000	7.196000
H	-1.769000	-0.815000	6.523000
H	-5.873000	-1.087000	4.099000
H	-4.158000	-0.926000	5.856000

CBH

subsystemA:1-56; subsystemB: 57-112

112

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	1.211000	1.588000	2.119000
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	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	21.613000	13.541000	-2.151000
H	20.173000	14.321000	-2.828000
H	20.066000	11.821000	-3.122000
H	20.231000	11.601000	-1.385000
H	18.070000	12.822000	-1.023000
H	17.907000	13.049000	-2.760000
H	17.848000	10.558000	-3.080000
H	17.996000	10.332000	-1.342000
H	15.829000	11.554000	-0.999000
H	15.687000	11.788000	-2.737000
H	15.630000	9.299000	-3.068000
H	15.759000	9.066000	-1.329000
H	13.588000	10.287000	-1.006000
H	13.465000	10.526000	-2.745000
H	13.412000	8.039000	-3.084000
H	13.527000	7.799000	-1.345000
H	11.352000	9.016000	-1.035000
H	11.240000	9.256000	-2.774000
H	11.194000	6.770000	-3.117000
H	11.307000	6.527000	-1.378000
H	9.128000	7.738000	-1.069000
H	9.015000	7.976000	-2.808000
H	8.972000	5.490000	-3.149000
H	9.096000	5.248000	-1.410000
H	6.916000	6.453000	-1.089000
H	6.789000	6.685000	-2.828000
H	6.751000	4.200000	-3.162000
H	6.894000	3.961000	-1.425000

H 4.712000 5.157000 -1.082000
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 4.567000 5.387000 -2.821000
H 20.324000 14.109000 -1.076000

GCGC
subsystemA:1-29; subsystemB: 30-58

58

C -1.598228 -2.949036 3.250000
C -4.000540 -2.906527 3.250000
C -4.010728 -1.569866 3.250000
C -2.719298 -0.918718 3.250000
N -2.830899 -3.586836 3.250000
N -1.594926 -1.599866 3.250000
N -2.653199 0.402428 3.250000
O -0.598071 -3.629523 3.250000
H -2.806641 -4.581039 3.250000
H -4.897292 -3.497190 3.250000
H -4.923580 -1.008975 3.250000
H -3.479494 0.950075 3.250000
H -1.758104 0.864659 3.250000
C 1.069242 1.108675 3.250000
C 2.285426 -1.022118 3.250000
C 3.455046 0.844410 3.250000
C 2.372412 1.689149 3.250000
C 4.058669 2.949205 3.250000
N 1.142384 -0.283906 3.250000
N 3.479383 -0.500070 3.250000
N 2.783809 3.007658 3.250000
N 4.536778 1.657659 3.250000
N 2.134562 -2.349372 3.250000
O -0.013009 1.651379 3.250000
H 0.255022 -0.761450 3.250000
H 4.722994 3.789401 3.250000
H 5.483879 1.360580 3.250000
H 2.960976 -2.896653 3.250000
H 1.238164 -2.794426 3.250000
C -1.516698 0.268452 0.000000
C -1.248162 -2.170251 0.000000
C -3.291523 -1.347683 0.000000
C -2.912179 -0.027919 0.000000

C	-5.017031	0.000331	0.000000
N	-0.757332	-0.901161	0.000000
N	-2.520946	-2.449695	0.000000
N	-4.020006	0.796964	0.000000
N	-4.644678	-1.325577	0.000000
N	-0.345970	-3.155346	0.000000
O	-0.960132	1.343640	0.000000
H	0.241252	-0.765924	0.000000
H	-6.048336	0.289583	0.000000
H	-5.236280	-2.122611	0.000000
H	-0.692870	-4.083860	0.000000
H	0.640827	-2.988513	0.000000
C	3.026394	-1.446405	0.000000
C	4.944918	0.000029	0.000000
C	4.167491	1.087399	0.000000
C	2.739967	0.855105	0.000000
N	4.398535	-1.237850	0.000000
N	2.230700	-0.356844	0.000000
N	1.909942	1.885083	0.000000
O	2.617230	-2.584808	0.000000
H	4.963288	-2.056436	0.000000
H	6.017589	0.049270	0.000000
H	4.576320	2.077730	0.000000
H	2.256529	2.813822	0.000000
H	0.914102	1.732911	0.000000

GGG

subsystemA:1-16; subsystemB: 17-48

48

N	6.392000	8.215000	35.830000
C	7.166000	7.124000	35.519000
N	6.952000	6.084000	36.266000
C	5.944000	6.488000	37.137000
C	5.338000	5.822000	38.204000
O	5.492000	4.688000	38.607000
N	4.395000	6.661000	38.871000
C	4.080000	7.958000	38.559000
N	3.196000	8.624000	39.322000
N	4.632000	8.592000	37.526000
C	5.581000	7.803000	36.882000
H	6.360000	9.115000	35.370000
H	3.905000	6.201000	39.663000
H	7.894000	7.170000	34.719000
H	2.998000	9.576000	39.055000
H	2.769000	8.213000	40.159000

N 6.665000 8.853000 40.553000
C 7.635000 8.238000 39.879000
N 7.807000 6.982000 40.232000
C 6.865000 6.766000 41.223000
C 6.571000 5.612000 41.963000
O 7.103000 4.485000 41.897000
N 5.522000 5.859000 42.882000
C 4.907000 7.088000 43.075000
N 4.067000 7.176000 44.053000
N 5.151000 8.148000 42.354000
C 6.159000 7.913000 41.451000
H 6.292000 9.782000 40.410000
H 5.265000 5.069000 43.495000
H 8.202000 8.733000 39.102000
H 3.862000 6.413000 44.701000
H 3.576000 8.051000 44.161000
N 6.807000 8.076000 45.803000
C 7.701000 8.119000 44.791000
N 8.170000 6.960000 44.522000
C 7.597000 6.103000 45.431000
C 7.781000 4.665000 45.638000
O 8.506000 3.870000 44.936000
N 7.042000 4.200000 46.733000
C 6.203000 5.003000 47.484000
N 5.593000 4.383000 48.504000
N 6.020000 6.303000 47.246000
C 6.754000 6.770000 46.226000
H 6.271000 8.839000 46.195000
H 7.067000 3.177000 46.909000
H 7.925000 9.033000 44.257000
H 5.654000 3.371000 48.664000
H 4.916000 4.925000 49.020000

PHE

subsystemA:1-29; subsystemB: 30-87

87

C -4.127538 -8.273547 -15.224887
C -4.997304 -7.682800 -16.150263
C -6.056402 -8.450504 -16.653267
C -6.260255 -9.759694 -16.217693
C -5.400847 -10.326978 -15.275882
C -4.326629 -9.582890 -14.788046
C -4.820615 -6.240143 -16.558153
C -5.697086 -5.258939 -15.718866
C -5.414712 -3.817756 -16.179678
C -7.938789 -6.041588 -14.998100

C	-9.397268	-6.178134	-15.394150
N	-4.474220	-3.160081	-15.461406
N	-7.120764	-5.492756	-15.925400
O	-7.534296	-6.441358	-13.892727
O	-5.989625	-3.354134	-17.169427
H	-9.632640	-7.243384	-15.485983
H	-4.267606	-2.202197	-15.716412
H	-10.022254	-5.766658	-14.596809
H	-9.640526	-5.679899	-16.336960
H	-7.504470	-5.059242	-16.761218
H	-5.482756	-5.389188	-14.656556
H	-5.074894	-6.099082	-17.615077
H	-3.776712	-5.936398	-16.426167
H	-6.727090	-8.012860	-17.388869
H	-3.288316	-7.699108	-14.838954
H	-7.089663	-10.338585	-16.615527
H	-3.650657	-10.017818	-14.057445
H	-5.563781	-11.342466	-14.927066
H	-4.170184	-3.512149	-14.551471
C	-3.969850	-4.923724	-11.758047
C	-4.851107	-6.024975	-11.146590
C	-7.159686	-5.649346	-10.366778
C	-4.456498	-7.385828	-11.789262
C	-5.180606	-8.557111	-11.171394
C	-6.442163	-8.946222	-11.643416
C	-7.132821	-9.992330	-11.029697
C	-6.572851	-10.666029	-9.942816
C	-5.309207	-10.298036	-9.478795
C	-4.619419	-9.253655	-10.093286
C	-8.609740	-5.527168	-10.792593
C	-3.166800	-5.116687	-7.134488
C	-4.301976	-5.956929	-6.502813
C	-5.942867	-4.271725	-5.766063
C	-4.394794	-7.358398	-7.127439
C	-5.394350	-8.255824	-6.432851
C	-5.024113	-9.002966	-5.307343
C	-5.943664	-9.832048	-4.664863
C	-7.251823	-9.925929	-5.143321
C	-7.630287	-9.186551	-6.264839
C	-6.708502	-8.359150	-6.905830
C	-7.324477	-3.687297	-5.987531
N	-6.261056	-5.743958	-11.375104
N	-2.982201	-4.469610	-10.962843
N	-2.761063	-4.089719	-6.351989
N	-5.565673	-5.231404	-6.648939
O	-4.139587	-4.532793	-12.924495
O	-6.836362	-5.645194	-9.164767
O	-2.683774	-5.362826	-8.250422
O	-5.211745	-3.909627	-4.825979

H	-7.975253	-4.021614	-5.172459
H	-2.120934	-3.406650	-6.739461
H	-7.266046	-2.596549	-5.941347
H	-2.336485	-3.787525	-11.341477
H	-9.199942	-6.249716	-10.222306
H	-8.969421	-4.524949	-10.536114
H	-7.761900	-3.997789	-6.939896
H	-6.111309	-5.396827	-7.500547
H	-4.110491	-6.038844	-5.427481
H	-4.657155	-7.265591	-8.183670
H	-3.395714	-7.804539	-7.083216
H	-7.002167	-7.795141	-7.786922
H	-4.003663	-8.938422	-4.933935
H	-8.644799	-9.259768	-6.647536
H	-5.638534	-10.408023	-3.795133
H	-7.968855	-10.574257	-4.647102
H	-3.347789	-3.835840	-5.549570
H	-8.746692	-5.704229	-11.861657
H	-6.615231	-5.861317	-12.329945
H	-4.707388	-6.061012	-10.065901
H	-4.678428	-7.324391	-12.858505
H	-3.372769	-7.507198	-11.678320
H	-6.878366	-8.426737	-12.492101
H	-3.635739	-8.967934	-9.727744
H	-8.111024	-10.283061	-11.403870
H	-4.867631	-10.814273	-8.631675
H	-7.115799	-11.472677	-9.458594
H	-2.854914	-4.784767	-9.994774