

Cartesian Coordinates of Complexes

A-T

7	-3.682823000	-1.817515000	-0.000395000
6	-2.418162000	-1.381148000	-0.000304000
6	-2.206511000	0.012134000	0.000214000
6	-3.339154000	0.810040000	0.000343000
7	-4.605715000	0.397070000	0.000207000
6	-4.676982000	-0.926885000	-0.000145000
7	-2.861128000	2.098238000	0.000575000
6	-1.498211000	2.022114000	0.000474000
7	-1.069347000	0.791411000	0.000274000
7	-1.416699000	-2.268557000	-0.000844000
1	-5.676360000	-1.348508000	-0.000196000
1	-0.855926000	2.890104000	0.000631000
1	-1.659925000	-3.243929000	-0.000862000
1	-0.439579000	-1.996588000	-0.000260000
1	-3.422575000	2.933117000	0.000799000
6	4.371040000	-2.246520000	0.000769000
6	3.725783000	-0.899854000	0.000291000
6	4.395033000	0.262574000	-0.000014000
7	3.761982000	1.481356000	-0.000631000
1	4.284819000	2.341819000	0.000046000
6	2.389283000	1.620456000	-0.000504000
8	1.840926000	2.701627000	-0.000473000
7	1.716772000	0.428067000	-0.000477000
1	0.677313000	0.500009000	-0.000338000
6	2.264634000	-0.836809000	0.000090000
8	1.545860000	-1.823048000	0.000372000
1	4.061199000	-2.818163000	0.876387000
1	4.061812000	-2.818517000	-0.874836000
1	5.456615000	-2.158817000	0.001138000
1	5.476508000	0.303750000	0.000052000

Cl-1

7	4.142127000	-1.315788000	-0.028920000
6	2.832482000	-1.099144000	-0.143077000
6	2.342313000	0.213486000	-0.035207000
6	3.327165000	1.185429000	0.156922000
7	4.638973000	0.999376000	0.260321000
6	4.960236000	-0.280597000	0.158710000
7	2.647770000	2.371249000	0.205076000
6	1.321596000	2.082052000	0.045004000
7	1.092398000	0.808652000	-0.099668000
7	2.082695000	-2.204437000	-0.423941000
1	6.013714000	-0.523265000	0.239592000

1	0.550870000	2.836909000	0.037921000
1	2.550968000	-3.081730000	-0.244242000
1	3.062728000	3.279285000	0.329154000
6	-5.058256000	-1.670179000	0.282413000
6	-4.164783000	-0.484586000	0.123436000
6	-4.595484000	0.774604000	-0.019302000
7	-3.730938000	1.832813000	-0.160074000
1	-4.069485000	2.775817000	-0.258177000
6	-2.360755000	1.701367000	-0.167724000
8	-1.627951000	2.661481000	-0.281200000
7	-1.920375000	0.408275000	-0.035237000
6	-2.718365000	-0.721064000	0.124557000
8	-2.231793000	-1.824402000	0.255419000
1	-4.878821000	-2.392187000	-0.514955000
1	-4.849073000	-2.181744000	1.222541000
1	-6.105978000	-1.373411000	0.264406000
1	-5.646907000	1.030228000	-0.030641000
17	0.421310000	-2.227665000	-0.115375000
1	-0.897771000	0.294584000	-0.055274000

Cl-2

7	-3.666770000	2.100608000	-0.000141000
6	-2.609862000	1.279377000	-0.000446000
6	-2.854261000	-0.110556000	-0.000125000
6	-4.188712000	-0.493100000	0.000350000
7	-5.254819000	0.306184000	0.000611000
6	-4.895344000	1.581505000	0.000365000
7	-4.161131000	-1.864101000	0.000423000
6	-2.843984000	-2.234481000	-0.000078000
7	-2.030842000	-1.220069000	-0.000364000
7	-1.383448000	1.815725000	-0.001133000
1	-5.704390000	2.304105000	0.000528000
1	-2.543533000	-3.270399000	-0.000126000
1	-1.309624000	2.818189000	-0.000859000
1	-4.966274000	-2.467064000	0.000814000
6	4.291871000	2.679576000	0.000485000
6	3.973084000	1.219930000	0.000282000
6	4.890132000	0.244363000	0.000221000
7	4.551268000	-1.083441000	-0.000099000
1	5.257542000	-1.801741000	0.000282000
6	3.257291000	-1.559553000	-0.000037000
8	2.991204000	-2.730658000	-0.000061000
7	2.307973000	-0.537827000	-0.000078000
6	2.560350000	0.845937000	0.000109000
8	1.650950000	1.643120000	0.000020000
1	3.861030000	3.164974000	-0.875778000

1	3.860129000	3.164885000	0.876349000
1	5.368957000	2.839630000	0.001040000
1	5.952074000	0.450949000	0.000321000
17	0.682545000	-1.006511000	-0.000173000
1	-0.535395000	1.269901000	-0.000604000

Cl-1,2

7	4.572233000	-1.502959000	0.089795000
6	3.310349000	-1.128227000	-0.118334000
6	2.990002000	0.240056000	-0.077139000
6	4.075028000	1.084772000	0.174673000
7	5.341737000	0.737283000	0.375830000
6	5.502248000	-0.575145000	0.314589000
7	3.551720000	2.348351000	0.157398000
6	2.213392000	2.218396000	-0.099041000
7	1.837042000	0.984965000	-0.247111000
7	2.451811000	-2.146624000	-0.420197000
1	6.508299000	-0.947487000	0.470957000
1	1.557840000	3.073544000	-0.162508000
1	2.816192000	-3.063457000	-0.201072000
1	4.069194000	3.198341000	0.305610000
6	-4.955351000	-2.349442000	0.290794000
6	-4.451940000	-0.947863000	0.173145000
6	-5.234013000	0.137828000	0.153581000
7	-4.727272000	1.407480000	0.044535000
1	-5.333470000	2.211659000	0.033379000
6	-3.385218000	1.706641000	-0.055009000
8	-2.973470000	2.832653000	-0.146049000
7	-2.577039000	0.572423000	-0.037875000
6	-3.002935000	-0.768020000	0.073583000
8	-2.208285000	-1.675684000	0.083256000
1	-4.642534000	-2.940851000	-0.570280000
1	-4.537075000	-2.832273000	1.174544000
1	-6.042196000	-2.365737000	0.357524000
1	-6.311782000	0.074492000	0.223045000
17	0.784889000	-2.005844000	-0.185954000
17	-0.911443000	0.818527000	-0.158195000

Br-1

7	4.175702000	-1.009351000	0.010547000
6	2.861710000	-0.825704000	-0.129205000
6	2.343645000	0.479995000	-0.036201000
6	3.304666000	1.473201000	0.165926000
7	4.618641000	1.317429000	0.292308000
6	4.968124000	0.043888000	0.204811000
7	2.601285000	2.645578000	0.195983000

6	1.284108000	2.329005000	0.017199000
7	1.081856000	1.050657000	-0.123554000
7	2.144306000	-1.948319000	-0.417524000
1	6.025097000	-0.175880000	0.304870000
1	0.500092000	3.069304000	-0.004719000
1	2.650427000	-2.806284000	-0.247596000
1	2.996634000	3.561998000	0.321905000
6	-5.141094000	-1.428803000	0.324299000
6	-4.237186000	-0.253610000	0.146931000
6	-4.656915000	1.008256000	-0.006111000
7	-3.783203000	2.055182000	-0.164158000
1	-4.112587000	3.000487000	-0.272236000
6	-2.414502000	1.910929000	-0.180085000
8	-1.674154000	2.861583000	-0.310455000
7	-1.984177000	0.613580000	-0.034900000
6	-2.794385000	-0.503847000	0.139438000
8	-2.324851000	-1.616136000	0.276648000
1	-4.974768000	-2.160603000	-0.466901000
1	-4.931041000	-1.932672000	1.268332000
1	-6.185708000	-1.121278000	0.310255000
1	-5.705880000	1.273771000	-0.012803000
1	-0.962967000	0.494475000	-0.060501000
35	0.331510000	-2.046858000	-0.087516000

Br-2

7	-3.758521000	2.194623000	-0.000045000
6	-2.696631000	1.378859000	0.000197000
6	-2.939664000	-0.013817000	0.000030000
6	-4.274803000	-0.396541000	-0.000109000
7	-5.342387000	0.398969000	-0.000251000
6	-4.985682000	1.675164000	-0.000240000
7	-4.251386000	-1.768255000	0.000096000
6	-2.939240000	-2.145057000	0.000149000
7	-2.124422000	-1.131345000	0.000177000
7	-1.478023000	1.932006000	0.000552000
1	-5.795760000	2.396500000	-0.000466000
1	-2.639197000	-3.180929000	0.000172000
1	-1.425601000	2.936132000	0.000231000
1	-5.059579000	-2.367482000	0.000071000
6	4.263482000	2.821378000	0.000032000
6	3.960547000	1.358480000	-0.000046000
6	4.888235000	0.393168000	0.000011000
7	4.560581000	-0.937019000	-0.000003000
1	5.271685000	-1.650308000	0.000037000
6	3.267603000	-1.420085000	-0.000028000
8	3.018849000	-2.597663000	0.000098000

7	2.308152000	-0.415242000	-0.000189000
6	2.551195000	0.965803000	-0.000167000
8	1.638040000	1.762770000	-0.000057000
1	3.826725000	3.302271000	-0.875840000
1	3.826646000	3.302194000	0.875907000
1	5.338848000	2.993521000	0.000088000
1	5.948207000	0.610170000	0.000095000
35	0.517222000	-0.933925000	-0.000064000
1	-0.618091000	1.404193000	0.000300000

Br-1,2

7	4.723251000	-1.240645000	0.134118000
6	3.444687000	-0.926770000	-0.084942000
6	3.067857000	0.431137000	-0.048881000
6	4.118274000	1.319642000	0.200499000
7	5.397715000	1.029308000	0.408579000
6	5.613022000	-0.275466000	0.357350000
7	3.550016000	2.563778000	0.171286000
6	2.221065000	2.386156000	-0.087927000
7	1.888991000	1.137715000	-0.227739000
7	2.646221000	-1.988122000	-0.393607000
1	6.632823000	-0.605101000	0.520712000
1	1.535731000	3.216955000	-0.160039000
1	3.085191000	-2.877664000	-0.199947000
1	4.037412000	3.432303000	0.314599000
6	-4.907434000	-2.411635000	0.338094000
6	-4.484750000	-0.984325000	0.212164000
6	-5.327376000	0.055173000	0.190176000
7	-4.891487000	1.349152000	0.073441000
1	-5.540090000	2.119510000	0.059761000
6	-3.566254000	1.718504000	-0.031567000
8	-3.222977000	2.868007000	-0.129398000
7	-2.694083000	0.636056000	-0.011874000
6	-3.048842000	-0.719577000	0.106214000
8	-2.209875000	-1.591518000	0.117386000
1	-4.564857000	-2.988782000	-0.521332000
1	-4.459784000	-2.866038000	1.222544000
1	-5.991440000	-2.489066000	0.408931000
1	-6.399756000	-0.068153000	0.263545000
35	0.822619000	-1.990679000	-0.132418000
35	-0.879712000	0.989147000	-0.147558000

I-1

7	4.265773000	-0.768661000	0.034212000
6	2.936908000	-0.623853000	-0.048336000
6	2.403566000	0.685573000	-0.021825000

6	3.354235000	1.702437000	0.073416000
7	4.676931000	1.579272000	0.148145000
6	5.043440000	0.307416000	0.123090000
7	2.633752000	2.865169000	0.069646000
6	1.315089000	2.521884000	-0.023830000
7	1.127207000	1.234850000	-0.080369000
7	2.228717000	-1.767529000	-0.176664000
1	6.108503000	0.111506000	0.183578000
1	0.520864000	3.250738000	-0.046494000
1	2.785577000	-2.605934000	-0.101841000
1	3.021113000	3.791712000	0.125999000
6	-5.247634000	-1.173989000	0.160831000
6	-4.315103000	-0.010479000	0.077505000
6	-4.705196000	1.269219000	0.017027000
7	-3.807839000	2.303326000	-0.058762000
1	-4.115168000	3.261428000	-0.102007000
6	-2.442771000	2.129913000	-0.079390000
8	-1.679528000	3.066484000	-0.143783000
7	-2.041858000	0.812951000	-0.020235000
6	-2.880438000	-0.290960000	0.059307000
8	-2.446304000	-1.429485000	0.110966000
1	-5.094675000	-1.847130000	-0.683301000
1	-5.056548000	-1.752898000	1.064951000
1	-6.284127000	-0.840207000	0.165515000
1	-5.747964000	1.557866000	0.024773000
53	0.217746000	-1.917376000	-0.033344000
1	-1.022816000	0.679262000	-0.040001000

I-2

7	-3.924607000	2.265154000	0.000077000
6	-2.830964000	1.492328000	-0.000134000
6	-3.026637000	0.089501000	-0.000080000
6	-4.347975000	-0.338956000	0.000186000
7	-5.442503000	0.415919000	0.000395000
6	-5.132130000	1.704570000	0.000320000
7	-4.282903000	-1.710806000	0.000220000
6	-2.966522000	-2.052567000	-0.000024000
7	-2.185010000	-1.010772000	-0.000283000
7	-1.639764000	2.101151000	-0.000476000
1	-5.967071000	2.396725000	0.000485000
1	-2.629495000	-3.076802000	-0.000039000
1	-1.639568000	3.107052000	-0.000323000
1	-5.074225000	-2.332871000	0.000410000
6	4.412465000	2.883135000	0.000155000
6	4.079966000	1.426971000	0.000113000
6	4.988569000	0.443651000	0.000254000

7	4.629310000	-0.878196000	0.000255000
1	5.321285000	-1.609576000	0.000353000
6	3.319896000	-1.321060000	0.000104000
8	3.049794000	-2.499442000	0.000148000
7	2.380127000	-0.310429000	-0.000028000
6	2.662523000	1.055528000	-0.000113000
8	1.769588000	1.882235000	-0.000090000
1	3.984837000	3.373097000	-0.875336000
1	3.984712000	3.373087000	0.875593000
1	5.491187000	3.034825000	0.000237000
1	6.053235000	0.637539000	0.000394000
1	-0.756335000	1.612668000	-0.000377000
53	0.358088000	-0.829827000	-0.000145000

I-1,2

7	-4.887926000	1.033310000	0.054414000
6	-3.574800000	0.774771000	-0.027688000
6	-3.166583000	-0.583834000	-0.010907000
6	-4.216520000	-1.503292000	0.078256000
7	-5.520128000	-1.260464000	0.154015000
6	-5.765638000	0.040221000	0.136018000
7	-3.624123000	-2.736830000	0.065438000
6	-2.282234000	-2.533504000	-0.028304000
7	-1.958993000	-1.273578000	-0.076716000
7	-2.800987000	1.875727000	-0.145090000
1	-6.806986000	0.336909000	0.196370000
1	-1.579246000	-3.352146000	-0.056255000
1	-3.330009000	2.733627000	-0.088449000
1	-4.110761000	-3.616248000	0.114916000
6	4.855740000	2.518359000	0.125576000
6	4.529098000	1.061288000	0.082211000
6	5.441818000	0.081451000	0.074232000
7	5.090192000	-1.241085000	0.034134000
1	5.787096000	-1.968089000	0.028733000
6	3.786063000	-1.694220000	-0.001913000
8	3.520459000	-2.870454000	-0.036336000
7	2.839529000	-0.682578000	0.005381000
6	3.114961000	0.686950000	0.046013000
8	2.221784000	1.514725000	0.050487000
1	4.442825000	3.029051000	-0.744989000
1	4.411015000	2.984160000	1.005625000
1	5.933671000	2.672644000	0.149178000
1	6.505146000	0.280302000	0.099204000
53	-0.795657000	2.027702000	-0.034204000
53	0.843108000	-1.185156000	-0.046920000

G-C+

7	5.395976000	-0.786023000	0.002993000
8	0.990590000	-2.078841000	0.000102000
7	3.149021000	-1.356322000	0.000480000
6	4.115753000	-0.377733000	0.000363000
7	3.843002000	0.900882000	-0.000344000
6	2.525541000	1.158815000	-0.000255000
6	1.481557000	0.255327000	-0.000090000
6	1.770001000	-1.133355000	0.000024000
7	1.925230000	2.385060000	-0.000720000
6	0.572914000	2.182254000	-0.000899000
7	0.274659000	0.913649000	-0.000465000
1	5.664296000	-1.752694000	-0.008682000
1	6.111290000	-0.079135000	-0.002776000
1	3.418249000	-2.331368000	0.002303000
1	2.402442000	3.273361000	-0.000799000
1	-0.146719000	2.985774000	-0.001217000
8	-2.726307000	2.230948000	0.000387000
7	-1.780319000	-2.232931000	-0.001319000
7	-2.285573000	0.002731000	-0.000168000
6	-4.086942000	-1.554221000	-0.000229000
6	-3.130178000	1.100220000	0.000434000
7	-4.477750000	0.773837000	0.001217000
6	-4.931309000	-0.502796000	0.000641000
6	-2.684872000	-1.280449000	-0.000596000
1	-4.450124000	-2.568832000	-0.000658000
1	-5.114514000	1.558316000	0.001403000
1	-6.005759000	-0.625370000	0.001024000
1	-0.761781000	-2.058330000	-0.001012000
1	-2.085024000	-3.192914000	-0.001185000
1	-1.251135000	0.279772000	-0.000387000

Cl-1

7	-5.779922000	-0.222264000	-0.038109000
8	-1.640603000	-2.148452000	0.005558000
7	-3.629368000	-1.089222000	0.001684000
6	-4.450968000	0.004819000	-0.001348000
7	-3.998143000	1.228064000	0.001356000
6	-2.655604000	1.291188000	-0.001519000
6	-1.724964000	0.263506000	0.004200000
6	-2.225393000	-1.076429000	0.005199000
7	-1.921522000	2.437220000	-0.004693000
6	-0.605318000	2.080877000	-0.001490000
7	-0.439337000	0.786380000	0.003804000
1	-6.168759000	-1.124836000	0.168437000
1	-6.377776000	0.582132000	0.051446000

1	-4.025371000	-2.019450000	-0.027240000
1	-2.297653000	3.372210000	-0.009319000
1	0.191293000	2.805280000	-0.002947000
8	2.376925000	2.479221000	0.006858000
7	2.468502000	-2.108067000	-0.003531000
7	2.405310000	0.198654000	0.001695000
6	4.527887000	-0.915124000	-0.004948000
6	3.003210000	1.458405000	0.003475000
7	4.387549000	1.433479000	0.001002000
6	5.119356000	0.295031000	-0.003144000
6	3.101590000	-0.953474000	-0.002251000
1	5.102408000	-1.826832000	-0.008220000
1	4.829422000	2.342649000	0.002314000
1	6.193958000	0.415765000	-0.004881000
1	2.992333000	-2.971553000	-0.006648000
1	1.350208000	0.229841000	0.003390000
17	0.784064000	-2.223168000	0.000166000

Cl-2

7	-5.518608000	-1.749870000	-0.045743000
8	-0.944556000	-1.603467000	0.009088000
7	-3.206373000	-1.563080000	0.002173000
6	-4.433123000	-0.948580000	-0.003301000
7	-4.579757000	0.347141000	-0.001012000
6	-3.409814000	1.008921000	-0.002142000
6	-2.122535000	0.494108000	0.007032000
6	-1.962334000	-0.919831000	0.007864000
7	-3.249020000	2.360381000	-0.005763000
6	-1.901036000	2.609110000	0.000417000
7	-1.198685000	1.516606000	0.008149000
1	-5.463089000	-2.725794000	0.185090000
1	-6.412825000	-1.296790000	0.045185000
1	-3.150906000	-2.572107000	-0.031088000
1	-3.993802000	3.039610000	-0.012621000
1	-1.502819000	3.610893000	-0.001219000
8	3.795097000	2.151585000	-0.000429000
7	1.765518000	-1.976811000	0.002209000
7	2.788299000	0.093271000	0.001105000
6	4.159728000	-1.857003000	-0.004397000
6	3.899942000	0.966644000	-0.001547000
7	5.111639000	0.296774000	-0.005509000
6	5.237635000	-1.050730000	-0.006914000
6	2.861513000	-1.260656000	-0.000264000
1	4.257180000	-2.930291000	-0.005523000
1	5.922928000	0.900071000	-0.007545000
1	6.248446000	-1.434485000	-0.010143000

1	0.805581000	-1.594602000	0.005079000
1	1.853683000	-2.980807000	0.000807000
17	1.250609000	0.828034000	0.005468000

Cl-1,2

7	-6.183587000	-0.885699000	-0.044001000
8	-1.717345000	-1.892795000	0.006803000
7	-3.899732000	-1.286756000	0.001312000
6	-4.930366000	-0.385198000	-0.003078000
7	-4.747678000	0.906812000	0.000220000
6	-3.447767000	1.251942000	-0.001500000
6	-2.330143000	0.435058000	0.005890000
6	-2.524427000	-0.983396000	0.006293000
7	-2.960884000	2.525781000	-0.004739000
6	-1.597611000	2.440589000	0.000080000
7	-1.187327000	1.206208000	0.006382000
1	-6.374081000	-1.846038000	0.179926000
1	-6.934395000	-0.222481000	0.051609000
1	-4.098114000	-2.277807000	-0.030816000
1	-3.518884000	3.365125000	-0.010517000
1	-0.960655000	3.310604000	-0.001422000
8	3.275190000	2.525978000	0.004026000
7	2.545151000	-2.090560000	-0.002560000
7	2.842545000	0.271862000	0.000895000
6	4.715152000	-1.211405000	-0.005965000
6	3.694158000	1.412612000	0.001093000
7	5.043015000	1.110473000	-0.002362000
6	5.535962000	-0.147273000	-0.005839000
6	3.297211000	-0.997503000	-0.002384000
1	5.105738000	-2.216172000	-0.008659000
1	5.652637000	1.917074000	-0.002290000
1	6.612721000	-0.244292000	-0.008436000
1	3.047518000	-2.966544000	-0.005466000
17	1.150164000	0.694398000	0.004358000
17	0.871672000	-2.287594000	0.001283000

Br-1

7	-5.869576000	-0.089434000	-0.032705000
8	-1.712223000	-1.951123000	0.002294000
7	-3.703416000	-0.916183000	-0.000016000
6	-4.546768000	0.162600000	-0.000913000
7	-4.114693000	1.393308000	0.002419000
6	-2.775200000	1.481740000	-0.000499000
6	-1.823958000	0.468330000	0.003284000
6	-2.306606000	-0.873072000	0.002987000
7	-2.062453000	2.639204000	-0.002167000

6	-0.737687000	2.304493000	-0.000034000
7	-0.548201000	1.015772000	0.003302000
1	-6.244411000	-1.003744000	0.145360000
1	-6.485650000	0.702209000	0.045564000
1	-4.081001000	-1.854349000	-0.025409000
1	-2.455662000	3.567260000	-0.005181000
1	0.047736000	3.041999000	-0.000891000
8	2.268180000	2.750298000	0.003386000
7	2.517109000	-1.830575000	-0.001365000
7	2.387969000	0.474920000	0.001067000
6	4.543524000	-0.564309000	-0.002736000
6	2.935983000	1.754493000	0.001569000
7	4.318680000	1.780491000	-0.000201000
6	5.089960000	0.665575000	-0.002281000
6	3.116762000	-0.664267000	-0.001003000
1	5.152733000	-1.453224000	-0.004399000
1	4.728956000	2.703916000	0.000094000
1	6.159465000	0.824721000	-0.003552000
1	3.083522000	-2.666630000	-0.003165000
1	1.344488000	0.468538000	0.002335000
35	0.652805000	-2.011718000	0.000264000

Br-2

7	5.709075000	1.697030000	-0.021864000
8	1.129528000	1.769909000	0.002770000
7	3.392150000	1.628411000	0.001087000
6	4.587945000	0.955720000	-0.000900000
7	4.673178000	-0.348630000	0.000716000
6	3.475148000	-0.952268000	-0.000631000
6	2.217573000	-0.376458000	0.002780000
6	2.112900000	1.049564000	0.002968000
7	3.253378000	-2.299895000	-0.002585000
6	1.904608000	-2.498806000	-0.000808000
7	1.260562000	-1.367652000	0.002338000
1	5.703484000	2.694476000	0.089176000
1	6.587377000	1.208904000	0.026509000
1	3.384466000	2.639645000	-0.015289000
1	3.969182000	-3.010534000	-0.005286000
1	1.452777000	-3.477222000	-0.001998000
8	-3.700595000	-2.027240000	0.000055000
7	-1.744732000	2.134824000	0.000230000
7	-2.718464000	0.037682000	0.000140000
6	-4.129320000	1.968037000	-0.001796000
6	-3.810046000	-0.837349000	-0.000566000
7	-5.043352000	-0.197498000	-0.002049000
6	-5.195804000	1.145436000	-0.002573000

6	-2.826207000	1.379438000	-0.000436000
1	-4.242399000	3.039853000	-0.002227000
1	-5.840708000	-0.818281000	-0.002558000
1	-6.212941000	1.512236000	-0.003664000
1	-0.788076000	1.772960000	0.001208000
1	-1.858412000	3.135079000	-0.000342000
35	-0.945130000	-0.760808000	0.001645000

Br-1,2

7	6.295085000	1.043970000	0.001088000
8	1.763583000	1.766982000	0.001892000
7	3.995746000	1.319634000	0.001652000
6	5.079683000	0.481598000	0.000638000
7	4.974440000	-0.826253000	-0.000812000
6	3.706091000	-1.249396000	-0.001208000
6	2.550275000	-0.497933000	-0.000199000
6	2.638063000	0.937014000	0.001202000
7	3.298887000	-2.560615000	-0.002883000
6	1.949860000	-2.591687000	-0.002848000
7	1.480096000	-1.367898000	-0.001323000
1	6.439726000	2.037412000	0.002889000
1	7.094762000	0.433287000	0.000515000
1	4.133765000	2.322202000	0.002398000
1	3.913187000	-3.362173000	-0.003945000
1	1.344588000	-3.483281000	-0.003828000
8	-2.749498000	-2.715217000	0.005253000
7	-2.917321000	1.909238000	-0.002464000
7	-2.732081000	-0.425683000	0.001039000
6	-4.897705000	0.654719000	-0.002865000
6	-3.349424000	-1.669697000	0.002787000
7	-4.743884000	-1.673823000	0.001532000
6	-5.491805000	-0.551140000	-0.001270000
6	-3.459306000	0.681862000	-0.001364000
1	-5.472923000	1.566328000	-0.004966000
1	-5.165057000	-2.591175000	0.002933000
1	-6.565499000	-0.678629000	-0.002069000
1	-3.539089000	2.701158000	-0.004476000
35	-0.408907000	-0.919808000	-0.000144000
35	-1.139873000	2.335200000	0.000125000

I-1

7	-5.960988000	0.056917000	-0.024978000
8	-1.800398000	-1.775155000	0.000980000
7	-3.786895000	-0.748453000	-0.000925000
6	-4.642908000	0.321704000	-0.001364000
7	-4.221182000	1.556634000	0.001693000

6	-2.885130000	1.660447000	0.000172000
6	-1.921863000	0.652073000	0.002654000
6	-2.398290000	-0.684033000	0.001567000
7	-2.182905000	2.821846000	0.000035000
6	-0.851873000	2.495778000	0.001909000
7	-0.651090000	1.211868000	0.003635000
1	-6.331233000	-0.867401000	0.102575000
1	-6.589085000	0.840666000	0.032706000
1	-4.153344000	-1.691459000	-0.019157000
1	-2.583879000	3.746764000	-0.001614000
1	-0.070352000	3.238707000	0.002062000
8	2.196588000	2.963833000	0.001118000
7	2.639062000	-1.602924000	-0.000548000
7	2.429714000	0.700335000	0.000424000
6	4.622219000	-0.245022000	-0.001736000
6	2.915033000	2.001354000	0.000256000
7	4.292992000	2.090949000	-0.000803000
6	5.112329000	1.006792000	-0.001774000
6	3.198684000	-0.422995000	-0.000606000
1	5.273544000	-1.103696000	-0.002558000
1	4.663336000	3.030530000	-0.000954000
1	6.173532000	1.213599000	-0.002645000
1	3.268006000	-2.393941000	-0.001503000
1	1.398603000	0.652481000	0.001384000
53	0.546815000	-1.877405000	0.000315000

I-2

7	5.872336000	1.803963000	-0.006793000
8	1.290130000	1.842712000	0.001028000
7	3.556718000	1.720377000	0.000614000
6	4.756971000	1.057392000	-0.000071000
7	4.852477000	-0.247821000	0.000170000
6	3.659916000	-0.859360000	-0.000514000
6	2.398924000	-0.295353000	0.000536000
6	2.276912000	1.134727000	0.000991000
7	3.452616000	-2.211781000	-0.001196000
6	2.111892000	-2.430515000	-0.000689000
7	1.455191000	-1.302942000	0.000350000
1	5.860968000	2.806661000	0.031119000
1	6.756081000	1.323811000	0.009572000
1	3.541119000	2.731758000	-0.004659000
1	4.177350000	-2.913790000	-0.002042000
1	1.667816000	-3.412403000	-0.001198000
8	-3.783848000	-1.898808000	0.000611000
7	-1.826421000	2.257978000	-0.000531000
7	-2.790594000	0.153865000	0.000091000

6	-4.206065000	2.090328000	-0.000965000
6	-3.885909000	-0.703905000	0.000168000
7	-5.124300000	-0.070455000	-0.000337000
6	-5.276196000	1.271761000	-0.000885000
6	-2.908003000	1.489106000	-0.000424000
1	-4.315505000	3.162574000	-0.001439000
1	-5.920832000	-0.691792000	-0.000228000
1	-6.292509000	1.640931000	-0.001261000
1	-1.942634000	3.257234000	-0.000821000
53	-0.800257000	-0.766070000	0.000423000
1	-0.875311000	1.898093000	-0.000050000

I-1,2

7	6.527324000	1.127490000	0.197757000
8	1.965185000	1.575777000	0.445136000
7	4.217188000	1.264650000	0.305109000
6	5.341105000	0.507675000	0.101689000
7	5.302601000	-0.770325000	-0.182874000
6	4.054430000	-1.252892000	-0.253074000
6	2.860961000	-0.586626000	-0.069417000
6	2.881227000	0.814341000	0.245081000
7	3.710351000	-2.550449000	-0.527436000
6	2.359483000	-2.641956000	-0.503265000
7	1.822779000	-1.479870000	-0.232944000
1	6.621004000	2.093192000	0.454224000
1	7.356557000	0.572530000	0.070495000
1	4.305705000	2.248881000	0.521233000
1	4.359678000	-3.301080000	-0.709951000
1	1.811112000	-3.552688000	-0.679469000
8	-2.673157000	-2.790614000	1.077889000
7	-2.822684000	1.473515000	-0.726804000
7	-2.654083000	-0.701979000	0.142405000
6	-4.773532000	0.150758000	-0.626685000
6	-3.269984000	-1.877969000	0.573432000
7	-4.645016000	-1.957374000	0.372610000
6	-5.366962000	-0.989140000	-0.226556000
6	-3.366779000	0.296427000	-0.381969000
1	-5.341731000	0.950644000	-1.073163000
1	-5.070235000	-2.816458000	0.690620000
1	-6.426179000	-1.172352000	-0.343573000
1	-3.476355000	2.125751000	-1.132436000
53	-1.205338000	2.424574000	0.048442000
53	-0.360788000	-1.081046000	-0.021505000

Watson-Crick

G-C

7	-2.364291000	1.096115000	0.000000000
8	1.177297000	-1.788596000	0.000000000
7	-0.651203000	-0.440919000	0.000000000
6	-1.995932000	-0.195837000	0.000000000
7	-2.903537000	-1.144630000	0.000000000
6	-2.358296000	-2.375358000	0.000000000
6	-1.020677000	-2.742410000	0.000000000
6	-0.045841000	-1.699708000	0.000000000
7	-3.041960000	-3.554157000	0.000000000
6	-2.100546000	-4.561816000	0.000000000
7	-0.885084000	-4.114064000	0.000000000
1	-1.690900000	1.858354000	0.000000000
1	-3.349283000	1.287435000	0.000000000
1	0.000000000	0.355220000	0.000000000
1	-4.043402000	-3.646456000	0.000000000
1	-2.387542000	-5.601341000	0.000000000
8	-0.385850000	3.254929000	0.000000000
7	3.059703000	0.280733000	0.000000000
7	1.319320000	1.745680000	0.000000000
6	3.572488000	2.625794000	0.000000000
6	0.810162000	2.998389000	0.000000000
7	1.720203000	4.059515000	0.000000000
6	3.061031000	3.869876000	0.000000000
6	2.629546000	1.536930000	0.000000000
1	4.636638000	2.451678000	0.000000000
1	1.315814000	4.982640000	0.000000000
1	3.674795000	4.760159000	0.000000000
1	2.384144000	-0.497751000	0.000000000
1	4.044479000	0.086336000	0.000000000

Cl-1,3

7	-1.221622000	2.447805000	0.514726000
8	-1.636029000	-2.128314000	0.029977000
7	-1.502408000	0.142789000	0.199542000
6	-2.049193000	1.386083000	0.234896000
7	-3.318615000	1.639065000	0.090441000
6	-4.052691000	0.514265000	-0.060193000
6	-3.625184000	-0.800395000	-0.096359000
6	-2.222874000	-1.068272000	0.038424000
7	-5.403198000	0.451809000	-0.220424000
6	-5.724351000	-0.881797000	-0.343407000
7	-4.687036000	-1.656749000	-0.274330000
1	-1.637958000	3.334470000	0.266477000
1	-0.494755000	0.047263000	0.285853000
1	-6.027918000	1.240070000	-0.238932000

1	-6.743308000	-1.206564000	-0.481390000
8	3.064900000	2.250734000	-0.351236000
7	2.690763000	-2.271883000	0.247975000
7	2.813131000	-0.003348000	-0.064056000
6	4.852977000	-1.316919000	-0.002269000
6	3.538459000	1.137547000	-0.239728000
7	4.935979000	1.000350000	-0.296566000
6	5.565991000	-0.189280000	-0.180661000
6	3.423514000	-1.153014000	0.048652000
1	5.326993000	-2.280163000	0.097821000
1	5.448106000	1.858232000	-0.430675000
1	6.645747000	-0.176651000	-0.239039000
1	3.124524000	-3.177769000	0.191975000
17	0.433406000	2.359587000	0.137441000
17	1.010051000	-2.279378000	0.176717000

Br-1,3

7	1.433088000	2.448433000	-0.426928000
8	1.827862000	-2.142410000	-0.185405000
7	1.712027000	0.133748000	-0.244584000
6	2.254130000	1.382355000	-0.187493000
7	3.521712000	1.616404000	0.019581000
6	4.245264000	0.482538000	0.130500000
6	3.814949000	-0.832443000	0.076972000
6	2.420105000	-1.080829000	-0.120196000
7	5.588726000	0.404670000	0.336306000
6	5.903000000	-0.935548000	0.395987000
7	4.868360000	-1.701766000	0.246092000
1	1.854295000	3.326265000	-0.159164000
1	0.709646000	0.045614000	-0.377746000
1	6.213516000	1.188378000	0.422594000
1	6.915841000	-1.271052000	0.552270000
8	-3.024104000	2.266440000	0.247133000
7	-2.641940000	-2.277130000	-0.078830000
7	-2.778448000	0.002464000	0.084154000
6	-4.812279000	-1.316615000	0.130162000
6	-3.501197000	1.143449000	0.207144000
7	-4.894173000	1.015509000	0.294384000
6	-5.523500000	-0.181183000	0.255291000
6	-3.381675000	-1.161162000	0.047169000
1	-5.288424000	-2.283467000	0.096263000
1	-5.405655000	1.879228000	0.386472000
1	-6.602189000	-0.165696000	0.329414000
1	-3.086668000	-3.179046000	-0.077675000
35	-0.398550000	2.362850000	-0.115085000
35	-0.799126000	-2.278054000	-0.138935000

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7	1.549808	2.481835	-0.017976
8	1.989175	-2.094464	-0.012001
7	1.874677	0.182854	-0.013714
6	2.407969	1.447295	-0.008335
7	3.70421	1.66741	0.003421
6	4.425647	0.533975	0.007829
6	3.990238	-0.78551	0.003136
6	2.588279	-1.017927	-0.00778
7	5.784594	0.448812	0.019416
6	6.101502	-0.894335	0.021165
7	5.05675	-1.658495	0.011759
53	-0.508079	2.373812	-0.004506
1	2.00165	3.382549	-0.005747
1	0.864611	0.094184	-0.022486
1	6.417245	1.230842	0.02565
1	7.125934	-1.231168	0.029639
8	-3.038573	2.188741	0.009905
7	-2.598092	-2.351479	0.000436
7	-2.784974	-0.07603	0.004985
6	-4.804893	-1.408281	0.009507
6	-3.515264	1.048204	0.00973
7	-4.903062	0.932721	0.014682
6	-5.525054	-0.272346	0.014373
6	-3.36896	-1.263594	0.004885
1	-5.280158	-2.376454	0.009203
1	-5.421219	1.797265	0.018011
1	-6.606107	-0.257907	0.018202
53	-0.534154	-2.295731	-0.005756
1	-3.052565	-3.250129	0.000029