Supporting information for: Artificial Neural Network Correction for Density-Functional Tight-Binding Molecular Dynamics Simulations

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Comparison of DFTB2 and DFTB3 for Potential Energy Surface (PES)

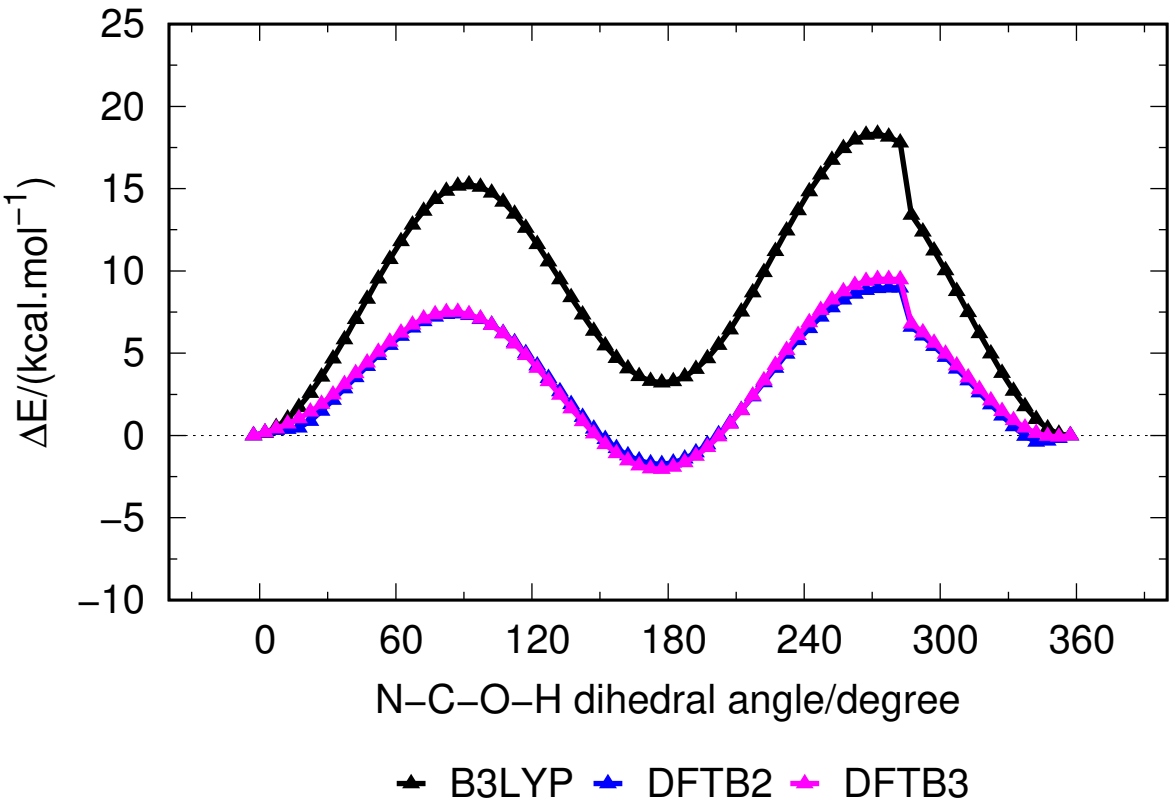

Figure S1: DFTB2, DFTB3 and B3LYP relative energy of glycine molecule as a function of the N-C-O-H dihedral angle in glycine.

Cartesian Coordinates of Glycine for the N-C-O-H Dihedral Angle Scan

Conformation 0

N 1.78490 0.11810 -0.04020

C 0.64060 -0.79990 0.05600

C -0.69370 -0.03680 0.00220

O -1.76400 -0.59830 -0.04600

O -0.55970 1.29780 0.03010

H 0.41290 1.46300 0.06080

H 0.61980 -1.55750 -0.73400

H 0.65680 -1.33790 1.00900

H 2.23770 0.08190 -0.94740

H 2.48720 -0.05180 0.67080

Conformation 1

N 1.78610 0.11690 -0.03900

C 0.63980 -0.79970 0.05070

C -0.69450 -0.03620 -0.00390

O -1.76540 -0.59770 -0.03770

O -0.55950 1.29820 0.02910

H 0.41240 1.46340 -0.02000

H 0.62720 -1.54540 -0.75010

H 0.64560 -1.35260 0.99540

H 2.30850 0.00700 -0.90130

H 2.43090 0.02050 0.73710

Conformation 2

N 1.78740 0.11670 -0.03870

C 0.64020 -0.79930 0.04570

C -0.69440 -0.03670 -0.00990

O -1.76530 -0.59880 -0.02880

O -0.56060 1.29830 0.02700

H 0.40250 1.46850 -0.10160

H 0.63680 -1.53040 -0.76790

H 0.63610 -1.36960 0.98040

H 2.38290 -0.07310 -0.83680

H 2.36230 0.10710 0.79630

Conformation 3

N 1.78880 0.11780 -0.03830

C 0.64250 -0.79800 0.04050

C -0.69320 -0.03880 -0.01560

O -1.76320 -0.60230 -0.02050

O -0.56410 1.29820 0.02570

H 0.38180 1.47890 -0.18110

H 0.64890 -1.51500 -0.78530

H 0.62910 -1.38540 0.96530

H 2.44930 -0.14320 -0.76140

H 2.29190 0.19370 0.83900

Conformation 4

N 1.79070 0.12020 -0.03820

C 0.64580 -0.79670 0.03480

C -0.69120 -0.04200 -0.02090

O -1.75960 -0.60740 -0.01260

O -0.56910 1.29780 0.02570

H 0.35150 1.49510 -0.25690

H 0.66070 -1.50060 -0.80220

H 0.62490 -1.39920 0.95050

H 2.50660 -0.20210 -0.67940

H 2.22390 0.27490 0.86630

Conformation 5

N 1.79330 0.12340 -0.03740

C 0.65060 -0.79440 0.02880

C -0.68880 -0.04620 -0.02560

O -1.75450 -0.61490 -0.00570

O -0.57660 1.29750 0.02760

H 0.31120 1.51540 -0.32750

H 0.67400 -1.48740 -0.81720

H 0.62320 -1.41030 0.93640

H 2.55000 -0.24290 -0.60400

H 2.16640 0.34370 0.88060

Conformation 6

N 1.79560 0.12690 -0.03720

C 0.65520 -0.79250 0.02260

C -0.68600 -0.05000 -0.02960

O -1.74920 -0.62220 0.00020

O -0.58300 1.29670 0.03060

H 0.26560 1.53700 -0.39350

H 0.68570 -1.47790 -0.82950

H 0.62280 -1.41670 0.92510

H 2.58410 -0.27500 -0.53220

H 2.11440 0.40350 0.88630

Conformation 7

N 1.79850 0.13110 -0.03680

C 0.66080 -0.79010 0.01640

C -0.68310 -0.05420 -0.03300

O -1.74290 -0.63100 0.00540

O -0.59090 1.29590 0.03460

H 0.21200 1.56040 -0.45450

H 0.69760 -1.46890 -0.84090

H 0.62450 -1.42230 0.91410

H 2.61100 -0.29690 -0.46730

H 2.06950 0.45620 0.88630

Conformation 8

N 1.80150 0.13550 -0.03680

C 0.66650 -0.78740 0.01070

C -0.68010 -0.05840 -0.03550

O -1.73640 -0.64020 0.00970

O -0.59870 1.29510 0.03930

H 0.15280 1.58400 -0.51060

H 0.70860 -1.46090 -0.85090

H 0.62750 -1.42640 0.90420

H 2.63210 -0.31140 -0.41030

H 2.03130 0.50200 0.88220

Conformation 9

N 1.80420 0.13990 -0.03700

C 0.67210 -0.78490 0.00550

C -0.67720 -0.06260 -0.03720

O -1.72990 -0.64930 0.01320

O -0.60580 1.29430 0.04440

H 0.08890 1.60660 -0.56190

H 0.71850 -1.45400 -0.85950

H 0.63190 -1.42970 0.89550

H 2.64860 -0.32020 -0.36070

H 1.99810 0.54240 0.87520

Conformation

N 1.80720 0.14470 -0.03800

C 0.67800 -0.78220 0.00090

C -0.67430 -0.06670 -0.03780

O -1.72330 -0.65870 0.01600

O -0.61280 1.29360 0.04970

H 0.02020 1.62780 -0.60840

H 0.72730 -1.44770 -0.86700

H 0.63750 -1.43200 0.88800

H 2.66220 -0.32580 -0.31580

H 1.96880 0.57970 0.86560

Conformation 11

N 1.80980 0.14940 -0.03960

C 0.68350 -0.77970 -0.00300

C -0.67130 -0.07050 -0.03760

O -1.71660 -0.66800 0.01810

O -0.61880 1.29270 0.05490

H -0.05230 1.64790 -0.64970

H 0.73450 -1.44140 -0.87390

H 0.64410 -1.43450 0.88110

H 2.67360 -0.32900 -0.27390

H 1.94160 0.61510 0.85340

Conformation 12

N 1.81270 0.15450 -0.04240

C 0.68940 -0.77700 -0.00570

C -0.66840 -0.07470 -0.03560

O -1.71040 -0.67720 0.01880

O -0.62480 1.29170 0.06020

H -0.12950 1.66540 -0.68600

H 0.74050 -1.43750 -0.87770

H 0.65280 -1.43420 0.87720

H 2.68300 -0.32870 -0.24060

H 1.92010 0.64680 0.83960

Conformation 13

N 1.81510 0.15910 -0.04590

C 0.69440 -0.77450 -0.00800

C -0.66560 -0.07810 -0.03300

O -1.70420 -0.68600 0.01940

O -0.62900 1.29100 0.06510

H -0.20790 1.68010 -0.71700

H 0.74470 -1.43270 -0.88210

H 0.66120 -1.43520 0.87310

H 2.69070 -0.32910 -0.20540

H 1.89780 0.67890 0.82280

Conformation 14

N 1.81740 0.16350 -0.05020

C 0.69920 -0.77210 -0.00920

C -0.66290 -0.08140 -0.02920

O -1.69850 -0.69410 0.01900

O -0.63210 1.29010 0.06980

H -0.28850 1.69200 -0.74240

H 0.74720 -1.42870 -0.88480

H 0.67070 -1.43520 0.87070

H 2.69690 -0.32750 -0.17710

H 1.87960 0.70800 0.80500

Conformation 15

N 1.81920 0.16720 -0.05610

C 0.70360 -0.77030 -0.00920

C -0.66020 -0.08460 -0.02360

O -1.69380 -0.70070 0.01730

O -0.63320 1.28920 0.07410

H -0.36970 1.69970 -0.76260

H 0.74720 -1.42750 -0.88470

H 0.68110 -1.43400 0.87100

H 2.70220 -0.32530 -0.14830

H 1.86060 0.73840 0.78270

Conformation 16

N 1.82110 0.17090 -0.06260

C 0.70790 -0.76860 -0.00790

C -0.65770 -0.08770 -0.01680

O -1.68960 -0.70690 0.01460

O -0.63380 1.28820 0.07800

H -0.45230 1.70460 -0.77710

H 0.74570 -1.42590 -0.88380

H 0.69310 -1.43290 0.87230

H 2.70700 -0.32110 -0.12580

H 1.84530 0.76630 0.75970

Conformation 17

N 1.82280 0.17390 -0.07010

C 0.71150 -0.76700 -0.00580

C -0.65530 -0.09020 -0.00880

O -1.68600 -0.71200 0.01110

O -0.63290 1.28710 0.08140

H -0.53480 1.70460 -0.78630

H 0.74250 -1.42560 -0.88110

H 0.70480 -1.43070 0.87540

H 2.71050 -0.31790 -0.10300

H 1.83060 0.79450 0.73370

Conformation 18

N 1.82450 0.17650 -0.07790

C 0.71470 -0.76520 -0.00310

C -0.65320 -0.09230 -0.00060

O -1.68250 -0.71670 0.00730

O -0.63120 1.28610 0.08410

H -0.61700 1.70260 -0.78910

H 0.73830 -1.42520 -0.87770

H 0.71630 -1.42820 0.87910

H 2.71340 -0.31410 -0.08340

H 1.81810 0.82020 0.70750

Conformation 19

N 1.82570 0.17880 -0.08640

C 0.71790 -0.76410 0.00050

C -0.65090 -0.09430 0.00870

O -1.67990 -0.71990 0.00250

O -0.62850 1.28430 0.08620

H -0.69840 1.69660 -0.78620

H 0.73270 -1.42640 -0.87250

H 0.72890 -1.42510 0.88430

H 2.71610 -0.30870 -0.06500

H 1.80550 0.84610 0.67870

Conformation 20

N 1.82730 0.18100 -0.09480

C 0.72080 -0.76240 0.00450

C -0.64890 -0.09590 0.01770

O -1.67740 -0.72290 -0.00210

O -0.62580 1.28270 0.08750

H -0.77920 1.68700 -0.77790

H 0.72710 -1.42750 -0.86660

H 0.74070 -1.42090 0.89010

H 2.71840 -0.30360 -0.04900

H 1.79570 0.86920 0.65100

Conformation 21

N 1.82880 0.18330 -0.10250

C 0.72360 -0.76060 0.00860

C -0.64700 -0.09710 0.02610

O -1.67490 -0.72560 -0.00670

O -0.62330 1.28060 0.08770

H -0.85860 1.67740 -0.76260

H 0.72190 -1.42810 -0.86060

H 0.75210 -1.41670 0.89590

H 2.72050 -0.29800 -0.03790

H 1.78880 0.88900 0.62610

Conformation 22

N 1.82980 0.18530 -0.10990

C 0.72610 -0.75900 0.01290

C -0.64510 -0.09830 0.03390

O -1.67290 -0.72720 -0.01110

O -0.62010 1.27830 0.08710

H -0.93540 1.66470 -0.74200

H 0.71730 -1.42960 -0.85390

H 0.76260 -1.41190 0.90230

H 2.72200 -0.29240 -0.02820

H 1.78270 0.90670 0.60260

Conformation 23

N 1.83160 0.18770 -0.11610

C 0.72890 -0.75680 0.01670

C -0.64340 -0.09890 0.03990

O -1.67070 -0.72960 -0.01450

O -0.61850 1.27570 0.08530

H -1.01060 1.65250 -0.71520

H 0.71440 -1.43020 -0.84770

H 0.77170 -1.40650 0.90810

H 2.72420 -0.28660 -0.02120

H 1.77930 0.92170 0.58310

Conformation 24

N 1.83330 0.18950 -0.12160

C 0.73110 -0.75450 0.02040

C -0.64190 -0.09950 0.04500

O -1.66920 -0.73090 -0.01760

O -0.61600 1.27310 0.08260

H -1.08150 1.63930 -0.68300

H 0.71180 -1.43120 -0.84130

H 0.77950 -1.40080 0.91410

H 2.72590 -0.28220 -0.01500

H 1.77720 0.93490 0.56510

Conformation 25

N 1.83480 0.19210 -0.12550

C 0.73360 -0.75230 0.02340

C -0.64030 -0.09980 0.04780

O -1.66720 -0.73270 -0.01950

O -0.61480 1.27030 0.07860

H -1.14940 1.62700 -0.64570

H 0.71190 -1.43190 -0.83580

H 0.78540 -1.39510 0.91940

H 2.72780 -0.27750 -0.01310

H 1.77720 0.94390 0.55400

Conformation 26

N 1.83630 0.19450 -0.12860

C 0.73580 -0.74990 0.02640

C -0.63890 -0.10000 0.04960

O -1.66600 -0.73380 -0.02110

O -0.61330 1.26760 0.07360

H -1.21260 1.61420 -0.60390

H 0.71270 -1.43270 -0.83010

H 0.79000 -1.38910 0.92480

H 2.72940 -0.27430 -0.01380

H 1.77950 0.95020 0.54660

Conformation 27

N 1.83770 0.19720 -0.13000

C 0.73790 -0.74740 0.02880

C -0.63760 -0.10000 0.04920

O -1.66460 -0.73540 -0.02150

O -0.61270 1.26500 0.06760

H -1.27140 1.60310 -0.55790

H 0.71560 -1.43310 -0.82530

H 0.79240 -1.38310 0.92960

H 2.73120 -0.27200 -0.01910

H 1.78470 0.95230 0.54620

Conformation 28

N 1.83920 0.19980 -0.13050

C 0.73990 -0.74480 0.03100

C -0.63640 -0.09990 0.04770

O -1.66380 -0.73650 -0.02150

O -0.61220 1.26240 0.06060

H -1.32520 1.59170 -0.50820

H 0.71960 -1.43360 -0.82050

H 0.79370 -1.37700 0.93430

H 2.73270 -0.27070 -0.02650

H 1.79160 0.95220 0.54910

Conformation 29

N 1.84050 0.20240 -0.12980

C 0.74160 -0.74240 0.03260

C -0.63530 -0.09980 0.04440

O -1.66280 -0.73780 -0.02060

O -0.61200 1.26020 0.05290

H -1.37340 1.58210 -0.45520

H 0.72470 -1.43410 -0.81650

H 0.79300 -1.37110 0.93850

H 2.73420 -0.26980 -0.03470

H 1.79890 0.95000 0.55560

Conformation 30

N 1.84190 0.20470 -0.12840

C 0.74320 -0.74020 0.03390

C -0.63430 -0.09970 0.04010

O -1.66240 -0.73860 -0.01930

O -0.61190 1.25810 0.04460

H -1.41590 1.57300 -0.39900

H 0.73080 -1.43510 -0.81260

H 0.79120 -1.36530 0.94250

H 2.73550 -0.26930 -0.04210

H 1.80580 0.94720 0.56300

Conformation 31

N 1.84300 0.20670 -0.12600

C 0.74450 -0.73840 0.03460

C -0.63340 -0.09960 0.03450

O -1.66200 -0.73930 -0.01730

O -0.61160 1.25640 0.03570

H -1.45220 1.56550 -0.34020

H 0.73740 -1.43650 -0.80920

H 0.78790 -1.35970 0.94600

H 2.73660 -0.26850 -0.04740

H 1.81120 0.94410 0.57100

Conformation 32

N 1.84420 0.20840 -0.12320

C 0.74560 -0.73670 0.03500

C -0.63260 -0.09960 0.02800

O -1.66180 -0.73980 -0.01500

O -0.61150 1.25480 0.02640

H -1.48230 1.55900 -0.27910

H 0.74480 -1.43840 -0.80590

H 0.78340 -1.35420 0.94930

H 2.73760 -0.26810 -0.05040

H 1.81550 0.94130 0.57870

Conformation 33

N 1.84510 0.20950 -0.11970

C 0.74640 -0.73560 0.03490

C -0.63190 -0.09970 0.02050

O -1.66170 -0.74010 -0.01220

O -0.61120 1.25370 0.01690

H -1.50580 1.55410 -0.21620

H 0.75230 -1.44090 -0.80300

H 0.77790 -1.34890 0.95210

H 2.73850 -0.26740 -0.05050

H 1.81750 0.93920 0.58560

Conformation 34

N 1.84610 0.21050 -0.11600

C 0.74710 -0.73450 0.03450

C -0.63130 -0.09980 0.01260

O -1.66160 -0.74040 -0.00930

O -0.61130 1.25280 0.00710

H -1.52330 1.55010 -0.15170

H 0.76020 -1.44380 -0.79990

H 0.77160 -1.34360 0.95490

H 2.73930 -0.26690 -0.04810

H 1.81820 0.93790 0.59170

Conformation 35

N 1.84680 0.21090 -0.11210

C 0.74740 -0.73400 0.03380

C -0.63100 -0.09990 0.00410

O -1.66160 -0.74050 -0.00600

O -0.61110 1.25230 -0.00280

H -1.53390 1.54770 -0.08630

H 0.76790 -1.44720 -0.79710

H 0.76450 -1.33860 0.95730

H 2.74000 -0.26620 -0.04270

H 1.81670 0.93760 0.59630

Conformation 36

N 1.84740 0.21110 -0.10810

C 0.74780 -0.73360 0.03310

C -0.63070 -0.10020 -0.00450

O -1.66150 -0.74070 -0.00280

O -0.61140 1.25200 -0.01270

H -1.53840 1.54610 -0.02030

H 0.77550 -1.45090 -0.79410

H 0.75720 -1.33370 0.95960

H 2.74060 -0.26540 -0.03560

H 1.81380 0.93800 0.59990

Conformation 37

N 1.84800 0.21070 -0.10410

C 0.74760 -0.73350 0.03210

C -0.63080 -0.10040 -0.01330

O -1.66150 -0.74080 0.00050

O -0.61140 1.25220 -0.02260

H -1.53580 1.54670 0.04590

H 0.78280 -1.45510 -0.79110

H 0.74900 -1.32900 0.96170

H 2.74080 -0.26540 -0.02570

H 1.80960 0.93970 0.60140

Conformation 38

N 1.84850 0.21010 -0.10040

C 0.74740 -0.73360 0.03120

C -0.63100 -0.10080 -0.02170

O -1.66130 -0.74090 0.00360

O -0.61200 1.25270 -0.03230

H -1.52740 1.54770 0.11190

H 0.78970 -1.45960 -0.78780

H 0.74110 -1.32420 0.96390

H 2.74110 -0.26500 -0.01390

H 1.80400 0.94250 0.60100

Conformation 39

N 1.84870 0.20900 -0.09710

C 0.74700 -0.73390 0.03030

C -0.63130 -0.10110 -0.02970

O -1.66110 -0.74110 0.00660

O -0.61270 1.25350 -0.04180

H -1.51230 1.55040 0.17730

H 0.79570 -1.46430 -0.78440

H 0.73320 -1.31970 0.96600

H 2.74090 -0.26480 -0.00090

H 1.79740 0.94600 0.59900

Conformation 40

N 1.84890 0.20760 -0.09420

C 0.74650 -0.73440 0.02960

C -0.63180 -0.10140 -0.03720

O -1.66080 -0.74150 0.00930

O -0.61380 1.25480 -0.05090

H -1.49120 1.55360 0.24160

H 0.80080 -1.46930 -0.78090

H 0.72580 -1.31530 0.96830

H 2.74060 -0.26460 0.01370

H 1.78990 0.95060 0.59480

Conformation 41

N 1.84930 0.20600 -0.09200

C 0.74590 -0.73490 0.02920

C -0.63250 -0.10190 -0.04360

O -1.66050 -0.74190 0.01150

O -0.61560 1.25620 -0.05960

H -1.46430 1.55840 0.30440

H 0.80540 -1.47440 -0.77670

H 0.71890 -1.31090 0.97090

H 2.74020 -0.26470 0.02800

H 1.78290 0.95570 0.58880

Conformation 42

N 1.84940 0.20390 -0.09040

C 0.74500 -0.73560 0.02900

C -0.63340 -0.10210 -0.04930

O -1.66000 -0.74250 0.01340

O -0.61750 1.25810 -0.06780

H -1.43130 1.56420 0.36520

H 0.80840 -1.47950 -0.77270

H 0.71250 -1.30680 0.97350

H 2.73930 -0.26490 0.04330

H 1.77530 0.96150 0.58070

Conformation 43

N 1.84960 0.20140 -0.08980

C 0.74410 -0.73660 0.02920

C -0.63430 -0.10250 -0.05360

O -1.65980 -0.74300 0.01460

O -0.61970 1.26030 -0.07540

H -1.39220 1.57120 0.42370

H 0.81020 -1.48520 -0.76800

H 0.70740 -1.30270 0.97670

H 2.73820 -0.26500 0.05980

H 1.76700 0.96860 0.56920

Conformation 44

N 1.84960 0.19850 -0.08990

C 0.74300 -0.73770 0.02980

C -0.63530 -0.10280 -0.05680

O -1.65960 -0.74350 0.01530

O -0.62240 1.26250 -0.08230

H -1.34750 1.57950 0.47920

H 0.81060 -1.49050 -0.76340

H 0.70300 -1.29910 0.98000

H 2.73690 -0.26490 0.07580

H 1.75900 0.97590 0.55570

Conformation 45

N 1.84970 0.19520 -0.09110

C 0.74180 -0.73890 0.03080

C -0.63630 -0.10300 -0.05850

O -1.65950 -0.74390 0.01540

O -0.62530 1.26500 -0.08840

H -1.29740 1.58900 0.53130

H 0.80940 -1.49600 -0.75840

H 0.69980 -1.29580 0.98380

H 2.73530 -0.26480 0.09160

H 1.75110 0.98380 0.53950

Conformation 46

N 1.84980 0.19130 -0.09330

C 0.74030 -0.74030 0.03230

C -0.63750 -0.10320 -0.05860

O -1.65980 -0.74410 0.01460

O -0.62830 1.26770 -0.09360

H -1.24160 1.59990 0.57970

H 0.80650 -1.50180 -0.75290

H 0.69790 -1.29260 0.98800

H 2.73340 -0.26470 0.10840

H 1.74330 0.99250 0.51970

Conformation 47

N 1.84970 0.18750 -0.09640

C 0.73880 -0.74180 0.03440

C -0.63870 -0.10320 -0.05720

O -1.66000 -0.74450 0.01320

O -0.63200 1.27040 -0.09800

H -1.18160 1.61170 0.62340

H 0.80230 -1.50690 -0.74740

H 0.69740 -1.28990 0.99270

H 2.73170 -0.26460 0.12040

H 1.73760 0.99970 0.50070

Conformation 48

N 1.84960 0.18300 -0.10030

C 0.73680 -0.74320 0.03690

C -0.64020 -0.10270 -0.05440

O -1.66020 -0.74480 0.01120

O -0.63560 1.27340 -0.10160

H -1.11680 1.62460 0.66220

H 0.79630 -1.51220 -0.74160

H 0.69750 -1.28720 0.99780

H 2.72960 -0.26530 0.13200

H 1.73300 1.00660 0.47990

Conformation 49

N 1.84970 0.17910 -0.10560

C 0.73580 -0.74460 0.04060

C -0.64110 -0.10320 -0.04910

O -1.66110 -0.74470 0.00760

O -0.64080 1.27560 -0.10410

H -1.04930 1.63860 0.69540

H 0.78950 -1.51700 -0.73500

H 0.70160 -1.28490 1.00390

H 2.72840 -0.26440 0.14000

H 1.72960 1.01400 0.45720

Conformation 50

N 1.84950 0.17450 -0.11110

C 0.73370 -0.74570 0.04440

C -0.64270 -0.10220 -0.04320

O -1.66140 -0.74510 0.00420

O -0.64560 1.27810 -0.10590

H -0.97800 1.65330 0.72240

H 0.78060 -1.52060 -0.72910

H 0.70460 -1.28300 1.00960

H 2.72700 -0.26620 0.14370

H 1.72950 1.01840 0.43790

Conformation 51

N 1.84930 0.17090 -0.11740

C 0.73220 -0.74630 0.04920

C -0.64410 -0.10150 -0.03560

O -1.66180 -0.74550 -0.00030

O -0.65200 1.28000 -0.10700

H -0.90560 1.66830 0.74260

H 0.77190 -1.52340 -0.72250

H 0.71010 -1.28120 1.01600

H 2.72680 -0.26900 0.13850

H 1.73390 1.02030 0.42410

Conformation 52

N 1.84860 0.16950 -0.12340

C 0.73100 -0.74540 0.05510

C -0.64590 -0.10030 -0.02720

O -1.66170 -0.74720 -0.00480

O -0.66060 1.28130 -0.10850

H -0.83430 1.68350 0.75440

H 0.76420 -1.52320 -0.71590

H 0.71690 -1.27930 1.02270

H 2.72870 -0.27870 0.10870

H 1.75180 1.01150 0.43320

Conformation 53

N 1.84750 0.17230 -0.12820

C 0.73070 -0.74160 0.06290

C -0.64840 -0.09850 -0.01840

O -1.66040 -0.75110 -0.00930

O -0.67330 1.28180 -0.11110

H -0.76770 1.69940 0.75660

H 0.75950 -1.51800 -0.70930

H 0.72540 -1.27690 1.02980

H 2.73180 -0.29750 0.03730

H 1.79430 0.98300 0.47890

Conformation 54

N 1.84660 0.17610 -0.13210

C 0.73070 -0.73700 0.07130

C -0.65110 -0.09630 -0.00910

O -1.65890 -0.75540 -0.01400

O -0.68720 1.28170 -0.11300

H -0.70270 1.71470 0.75180

H 0.75450 -1.51100 -0.70300

H 0.73490 -1.27500 1.03660

H 2.73110 -0.31520 -0.04930

H 1.84770 0.94340 0.53180

Conformation 55

N 1.84580 0.17940 -0.13510

C 0.73050 -0.73270 0.07960

C -0.65390 -0.09360 0.00020

O -1.65780 -0.75870 -0.01910

O -0.70030 1.28130 -0.11360

H -0.63730 1.72850 0.74180

H 0.74810 -1.50370 -0.69740

H 0.74430 -1.27400 1.04260

H 2.72520 -0.32790 -0.13800

H 1.90410 0.89850 0.57900

Conformation 56

N 1.84530 0.18370 -0.13540

C 0.73050 -0.72740 0.08830

C -0.65720 -0.09040 0.00910

O -1.65670 -0.76210 -0.02430

O -0.71400 1.28080 -0.11320

H -0.57470 1.73960 0.72660

H 0.74140 -1.49470 -0.69200

H 0.75350 -1.27340 1.04790

H 2.71040 -0.33470 -0.25140

H 1.97820 0.83410 0.63290

Conformation 57

N 1.84520 0.18860 -0.13090

C 0.73040 -0.72130 0.09820

C -0.66140 -0.08620 0.01760

O -1.65630 -0.76480 -0.03090

O -0.72760 1.28060 -0.11100

H -0.51460 1.74780 0.70850

H 0.73260 -1.48590 -0.68450

H 0.76230 -1.27160 1.05390

H 2.67480 -0.32160 -0.41500

H 2.08580 0.72920 0.69410

Conformation 58

N 1.81710 0.18260 -0.04260

C 0.71200 -0.75560 0.12070

C -0.65910 -0.08590 0.03420

O -1.67630 -0.71660 -0.10190

O -0.65500 1.28650 -0.02970

H -0.36450 1.68450 0.80420

H 0.67500 -1.58010 -0.60770

H 0.78710 -1.22440 1.11010

H 1.80590 0.61760 -0.96040

H 2.71010 -0.28580 0.07530

Conformation 59

N 1.81370 0.17810 -0.04750

C 0.70770 -0.75890 0.12010

C -0.66140 -0.08310 0.03830

O -1.68170 -0.70830 -0.10220

O -0.65180 1.28710 -0.02550

H -0.28260 1.67690 0.78130

H 0.66570 -1.58220 -0.60890

H 0.78680 -1.22780 1.10890

H 1.81800 0.59080 -0.97550

H 2.70620 -0.28340 0.09740

Conformation 60

N 1.81040 0.17270 -0.05080

C 0.70230 -0.76250 0.11870

C -0.66420 -0.07940 0.04100

O -1.68800 -0.69900 -0.10160

O -0.64600 1.28830 -0.02080

H -0.20040 1.66520 0.75360

H 0.65520 -1.58320 -0.61260

H 0.78410 -1.23370 1.10580

H 1.82990 0.56380 -0.98810

H 2.70120 -0.28390 0.11870

Conformation 61

N 1.80690 0.16730 -0.05350

C 0.69690 -0.76650 0.11610

C -0.66680 -0.07610 0.04260

O -1.69530 -0.68850 -0.10040

O -0.63920 1.28890 -0.01570

H -0.12090 1.65160 0.72000

H 0.64690 -1.58470 -0.61730

H 0.78000 -1.23980 1.10200

H 1.84540 0.53560 -0.99950

H 2.69550 -0.28160 0.14540

Conformation 62

N 1.80390 0.16160 -0.05480

C 0.69110 -0.77030 0.11270

C -0.66940 -0.07220 0.04270

O -1.70210 -0.67880 -0.09820

O -0.63230 1.29010 -0.01040

H -0.04520 1.63470 0.68220

H 0.63850 -1.58490 -0.62400

H 0.77310 -1.24700 1.09680

H 1.86190 0.50930 -1.00760

H 2.68950 -0.27940 0.17260

Conformation 63

N 1.80090 0.15600 -0.05540

C 0.68520 -0.77430 0.10870

C -0.67210 -0.06840 0.04200

O -1.70960 -0.66830 -0.09560

O -0.62430 1.29110 -0.00480

H 0.02730 1.61620 0.63910

H 0.63110 -1.58510 -0.63160

H 0.76520 -1.25450 1.09090

H 1.88040 0.48170 -1.01440

H 2.68230 -0.27610 0.20260

Conformation 64

N 1.79790 0.15040 -0.05510

C 0.67910 -0.77830 0.10400

C -0.67480 -0.06450 0.04030

O -1.71710 -0.65790 -0.09230

O -0.61570 1.29210 0.00090

H 0.09550 1.59610 0.59130

H 0.62480 -1.58490 -0.64030

H 0.75600 -1.26240 1.08430

H 1.90170 0.45260 -1.01950

H 2.67400 -0.27100 0.23630

Conformation 65

N 1.79480 0.14520 -0.05420

C 0.67300 -0.78230 0.09860

C -0.67740 -0.06070 0.03760

O -1.72480 -0.64730 -0.08840

O -0.60670 1.29280 0.00640

H 0.15900 1.57480 0.53910

H 0.61960 -1.58480 -0.64960

H 0.74570 -1.27020 1.07700

H 1.92650 0.42110 -1.02310

H 2.66370 -0.26300 0.27480

Conformation 66

N 1.79200 0.13980 -0.05270

C 0.66670 -0.78620 0.09280

C -0.68020 -0.05640 0.03410

O -1.73220 -0.63730 -0.08390

O -0.59730 1.29390 0.01180

H 0.21770 1.55300 0.48260

H 0.61520 -1.58370 -0.66010

H 0.73380 -1.27890 1.06900

H 1.95480 0.38700 -1.02460

H 2.65150 -0.25260 0.31730

Conformation 67

N 1.78930 0.13490 -0.05090

C 0.66080 -0.78990 0.08680

C -0.68280 -0.05250 0.03010

O -1.73940 -0.62770 -0.07900

O -0.58820 1.29470 0.01680

H 0.27010 1.53120 0.42170

H 0.61210 -1.58240 -0.67090

H 0.72170 -1.28770 1.06050

H 1.98760 0.34920 -1.02400

H 2.63650 -0.23670 0.36550

Conformation 68

N 1.78700 0.13040 -0.04880

C 0.65520 -0.79340 0.08050

C -0.68550 -0.04850 0.02530

O -1.74620 -0.61880 -0.07350

O -0.57950 1.29550 0.02140

H 0.31620 1.51030 0.35680

H 0.61030 -1.58030 -0.68240

H 0.70870 -1.29650 1.05160

H 2.02490 0.30750 -1.02030

H 2.61820 -0.21630 0.41800

Conformation 69

N 1.78530 0.12640 -0.04640

C 0.65010 -0.79610 0.07410

C -0.68800 -0.04470 0.02000

O -1.75220 -0.61120 -0.06750

O -0.57190 1.29620 0.02520

H 0.35420 1.49140 0.28810

H 0.61010 -1.57730 -0.69410

H 0.69530 -1.30560 1.04200

H 2.06740 0.26150 -1.01270

H 2.59580 -0.19020 0.47470

Conformation 70

N 1.78430 0.12280 -0.04400

C 0.64580 -0.79830 0.06780

C -0.69040 -0.04140 0.01440

O -1.75750 -0.60490 -0.06100

O -0.56550 1.29680 0.02810

H 0.38400 1.47700 0.21560

H 0.61140 -1.57330 -0.70610

H 0.68200 -1.31460 1.03230

H 2.11630 0.20910 -0.99970

H 2.56790 -0.15580 0.53620

Conformation 71

N 1.78430 0.12010 -0.04200

C 0.64270 -0.79940 0.06170

C -0.69230 -0.03870 0.00840

O -1.76140 -0.60070 -0.05370

O -0.56180 1.29740 0.02960

H 0.40320 1.46760 0.13950

H 0.61470 -1.56660 -0.71950

H 0.66910 -1.32540 1.02110

H 2.17430 0.14820 -0.97870

H 2.53160 -0.10920 0.60360

Conformation 72

N 1.78490 0.11800 -0.04020

C 0.64060 -0.79990 0.05600

C -0.69380 -0.03680 0.00220

O -1.76410 -0.59820 -0.04600

O -0.55960 1.29780 0.03010

H 0.41300 1.46280 0.06080

H 0.61990 -1.55770 -0.73380

H 0.65680 -1.33760 1.00910

H 2.23750 0.08210 -0.94750

H 2.48730 -0.05200 0.67060