# Supporting Information for Publication: "Optimal Solution to Torsional Coefficients Fitting Problem in Force Fields Parametrization"

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**1. The github repository containing *K_fit.py* program and its description:**
https://github.com/mysarapa/K_fit

**2. Sample of energy profiles for all dihedral angles comparing torsional coefficients derived from *K_fit.py* (algebraic approach) and *fit_dihedral.py* (Monte Carlo method) programs.**

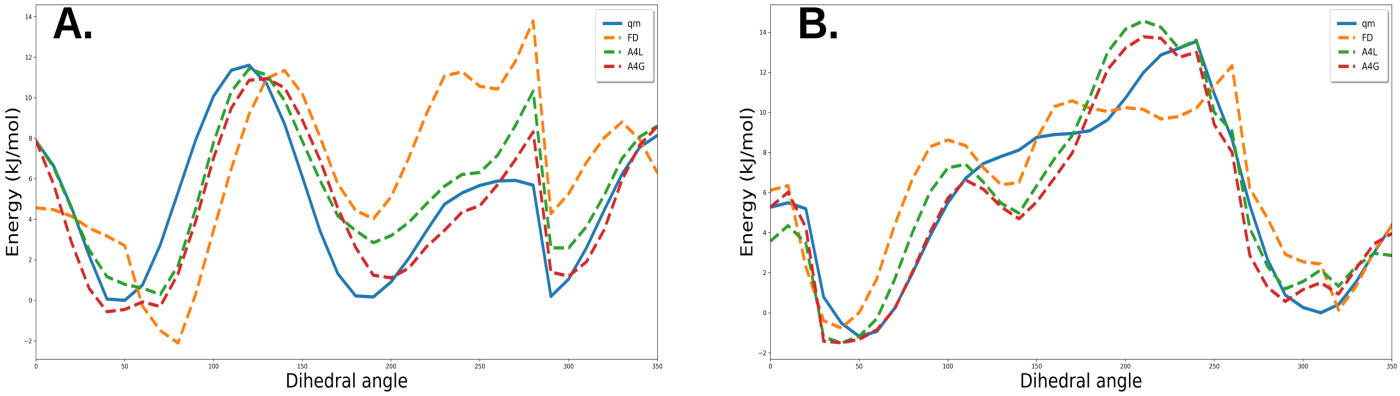


*Figure S1: Energy profiles for two dihedral angles in dimethyl phosphoric acid of CT-OS-P-OS type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

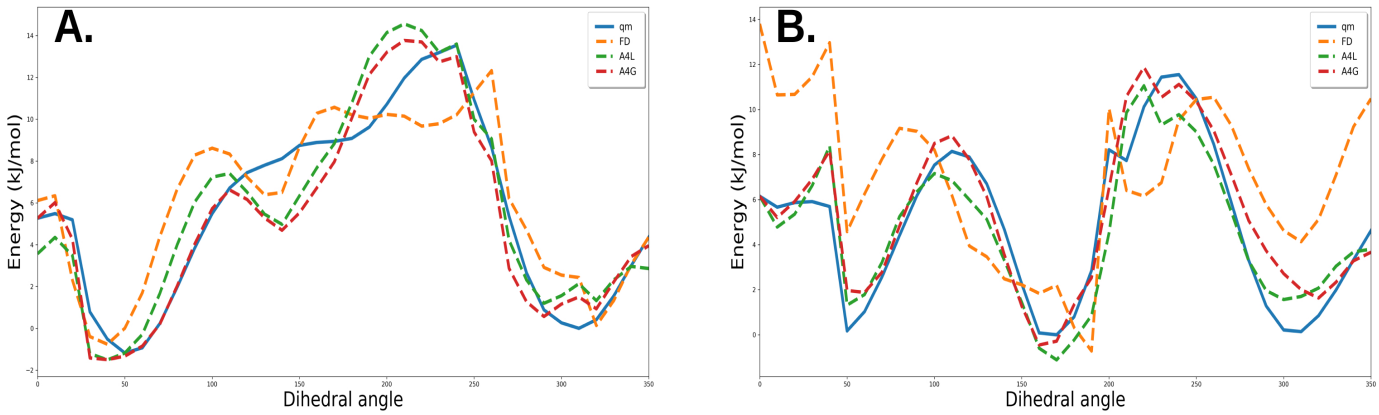


*Figure S2: Energy profiles for two dihedral angles in dimethyl phosphoric acid of CT-OS-P-O2 type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

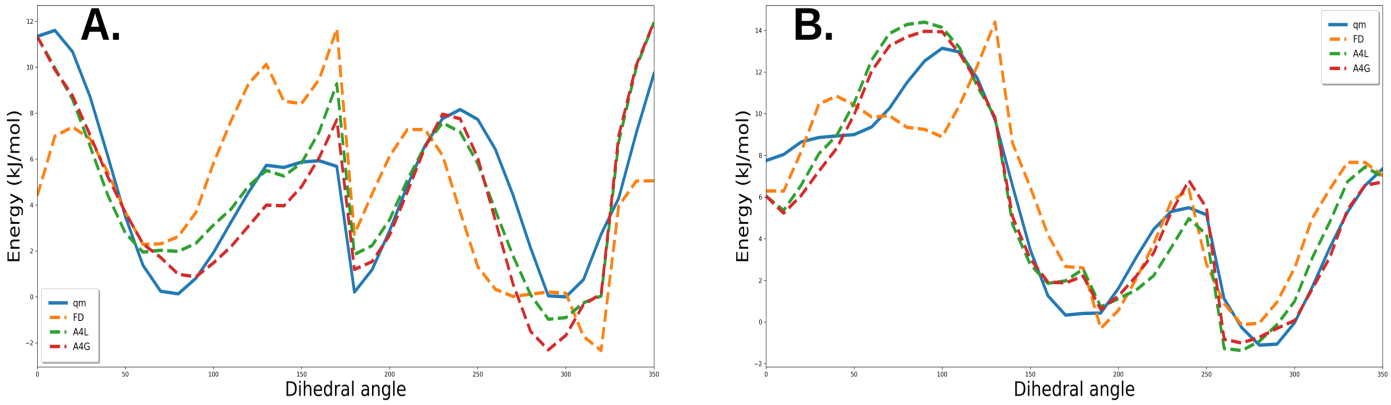


*Figure S3: Energy profiles for two dihedral angles in dimethyl phosphoric acid of CT-OS-P-OH type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

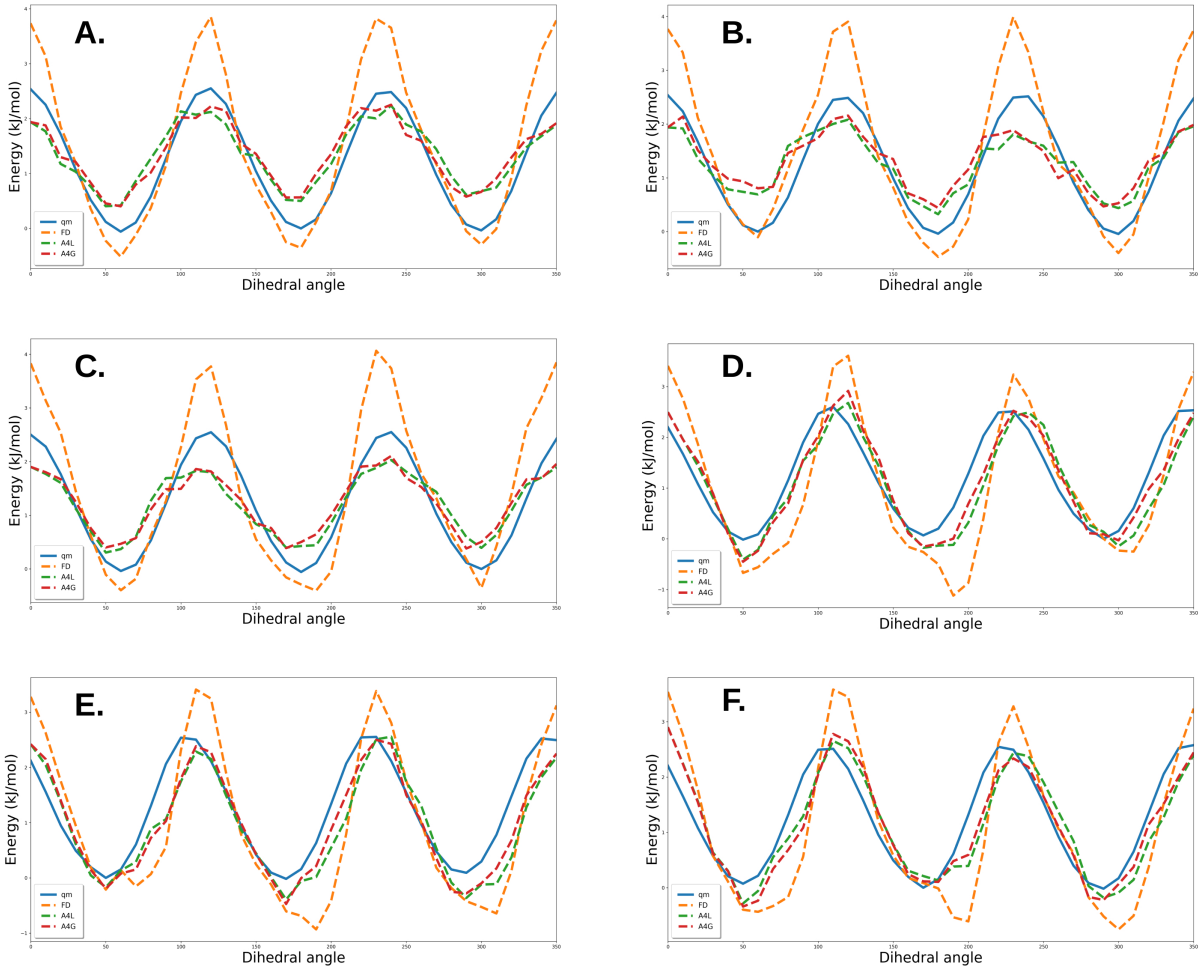


*Figure S4: Energy profiles for six dihedral angles in dimethyl phosphoric acid of HC-CT-OS-P type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

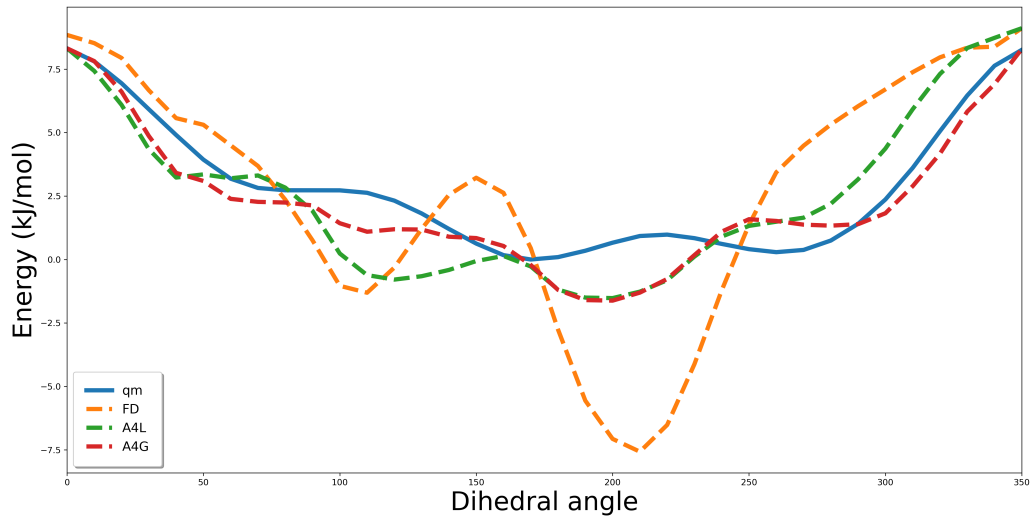


*Figure S5: Energy profiles for dihedral angle in dimethyl phosphoric acid of HO-OH-P-O2 type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

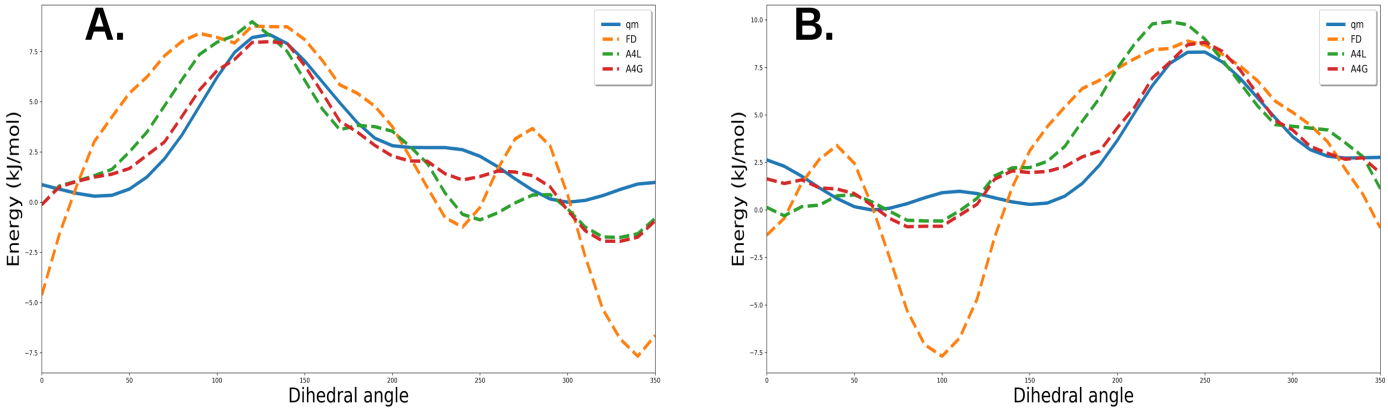


*Figure S6: Energy profiles for two dihedral angles in dimethyl phosphoric acid of HO-OH-P-OS type. FD refers to the results of fitting of Fourier coefficients based on the Monte Carlo simulations using fitdihedral.py program (Guvench, 2008). A4L (set 3 in Table 1) and A4G (set 4 in Table 1) were obtained using four-parameter algebraic method (local and global, respectively).*

**Table 1. Considered sets of parameters.**

| Set name | Set type | vdW parameters | Charges values | Minimization type | Number of parameters |
|---|---|---|---|---|---|
| Set1 | 1 | ORG | Q0 | L | 3 |
| Set2 | 1 | ORG | Q0 | G | 3 |
| Set3 | 1 | ORG | Q0 | L | 4 |
| Set4 | 1 | ORG | Q0 | G | 4 |
| Set5 | 2 | ORG | Qopls | L | 4 |
| Set6 | 2 | ORG | Qopls | L | 3 |
| Set7 | 2 | ORG | Qopls | G | 4 |
| Set8 | 2 | ORG | Qopls | G | 3 |
| Set9 | 3 | M | Q0 | L | 3 |
| Set10 | 3 | M | Q0 | G | 3 |
| Set11 | 3 | M | Q0 | L | 4 |
| Set12 | 3 | M | Q0 | G | 4 |
| Set13 | 4 | M | M | L | 3 |
| Set14 | 4 | M | M | G | 3 |
| Set15 | 4 | M | M | L | 4 |
| Set16 | 4 | M | M | G | 4 |

Summarizing, 16 sets of parameters were tested. There were 4 types of set differing in van der Waals parameters and partial charges. We performed both local (L) and global (G) minimization searching for 3 and 4 Fourier coefficients for each dihedral type.

**3. Sets of partial charges and van der Waals parameters used in the study:**

Q0

| nonbonded_atom type | bonded_atom_type | charges |
|---|---|---|
| opls_135 | CT | -0.045 |
| opls_140 | HC | 0.096 |
| opls_140 | HC | 0.096 |
| opls_140 | HC | 0.096 |
| opls_395 | OS | -0.331 |
| opls_393 | P | 0.945 |
| opls_394 | O2 | -0.550 |
| opls_268 | OH | -0.652 |
| opls_270 | HO | 0.433 |
| opls_395 | OS | -0.331 |
| opls_135 | CT | -0.045 |
| opls_140 | HC | 0.096 |
| opls_140 | HC | 0.096 |
| opls_140 | HC | 0.096 |

Qopls

| nonbonded_atom type | bonded_atom_type | charges |
|---|---|---|
| opls_135 | CT | 0.190 |
| opls_140 | HC | 0.060 |
| opls_140 | HC | 0.060 |
| opls_140 | HC | 0.060 |
| opls_395 | OS | -0.470 |
| opls_393 | P | 1.270 |
| opls_394 | O2 | -0.790 |
| opls_268 | OH | -0.700 |
| opls_270 | HO | 0.420 |
| opls_395 | OS | -0.470 |
| opls_135 | CT | 0.190 |
| opls_140 | HC | 0.060 |
| opls_140 | HC | 0.060 |
| opls_140 | HC | 0.060 |

M

| nonbonded_atom type | bonded_atom_type | charges |
|---|---|---|
| opls_443 | CT | 0.430 |
| opls_444 | HC | -0.030 |
| opls_444 | HC | -0.030 |
| opls_444 | HC | -0.030 |
| opls_442 | OS | -0.470 |
| opls_440 | P | 1.270 |
| opls_441 | O2 | -0.790 |
| opls_268 | OH | -0.640 |
| opls_270 | HO | 0.420 |
| opls_442 | OS | -0.470 |
| opls_443 | CT | 0.430 |
| opls_444 | HC | -0.030 |
| opls_444 | HC | -0.030 |
| opls_444 | HC | -0.030 |

vdW parameters - M

| | | sigma | epsilon |
|---|---|---|---|
| opls_440 | P | 3.74000e-01 | 0.58576 |
| opls_441 | O2 | 3.15000e-01 | 0.71128 |
| opls_442 | OS | 2.90000e-01 | 0.50208 |
| opls_268 | OH | 3.10000e-01 | 0.58576 |

**4. Sets of coefficients of Ryckeart Bellmans potential applied in the study:**

RB for DIHEDRALS

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assigned with *K_fit.py*

SET TYPE 1

SET1 (ORIG, Q0, L-3)----------RMSD= 1.3700 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 7.56 | -36.00 | -40.00 | 28.44 | 0.00 | 0.00 |
| CT | OS | P | OH | 3 | 7.92 | -48.68 | -37.64 | 40.76 | 0.00 | 0.00 |
| CT | OS | P | O2 | 3 | 38.59 | 35.77 | -25.82 | -74.36 | 0.00 | 0.00 |
| HC | CT | OS | P | 3 | -7.21 | 7.97 | -19.30 | -0.76 | 0.00 | 0.00 |
| HO | OH | P | O2 | 3 | -18.32 | 3.91 | -29.62 | 14.40 | 0.00 | 0.00 |
| HO | OH | P | OS | 3 | -16.96 | 29.12 | -39.66 | -12.16 | 0.00 | 0.00 |

SET2 (ORIG, Q0, G-3)----------RMSD= 1.1110 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 30.47 | -20.07 | -35.94 | -10.40 | 0.00 | 0.00 |
| CT | OS | P | OH | 3 | 32.06 | -32.22 | -31.96 | 0.16 | 0.00 | 0.00 |
| CT | OS | P | O2 | 3 | 35.59 | -33.47 | -23.24 | -2.12 | 0.00 | 0.00 |
| HC | CT | OS | P | 3 | 6.23 | -5.79 | -0.56 | -0.44 | 0.00 | 0.00 |
| HO | OH | P | O2 | 3 | -90.16 | 103.84 | -39.38 | -13.68 | 0.00 | 0.00 |
| HO | OH | P | OS | 3 | -89.18 | 86.90 | -55.58 | 2.28 | 0.00 | 0.00 |

SET3 (ORIG, Q0, L-4)----------RMSD= 1.2850 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 4.64 | -35.98 | -27.92 | 28.32 | -12.08 | 0.00 |
| CT | OS | P | OH | 3 | 6.92 | -45.52 | -26.82 | 36.00 | -10.40 | 0.00 |
| CT | OS | P | O2 | 3 | 31.77 | 32.35 | -2.78 | -69.80 | -22.72 | 0.00 |
| HC | CT | OS | P | 3 | -13.97 | 20.75 | -27.00 | -1.00 | 23.12 | 0.00 |
| HO | OH | P | O2 | 3 | -4.14 | -8.50 | -103.68 | 30.96 | 73.28 | 0.00 |
| HO | OH | P | OS | 3 | -2.91 | 36.29 | -86.64 | -21.72 | 46.64 | 0.00 |

SET4 (ORIG, Q0, G-4)----------RMSD= 1.0570 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 12.23 | -24.00 | -23.70 | 5.28 | -27.68 | 0.00 |
| CT | OS | P | OH | 3 | 12.29 | -33.03 | -13.42 | 12.36 | -33.52 | 0.00 |
| CT | OS | P | O2 | 3 | 19.43 | -5.05 | 20.86 | -27.48 | -52.40 | 0.00 |
| HC | CT | OS | P | 3 | 22.18 | -18.38 | -14.32 | -0.56 | 12.96 | 0.00 |
| HO | OH | P | O2 | 3 | -69.90 | 109.12 | -79.86 | -28.20 | 44.08 | 0.00 |
| HO | OH | P | OS | 3 | -78.86 | 77.34 | -80.88 | 9.08 | 30.24 | 0.00 |

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SET TYPE 2

SET5 (ORIG, Qopls, L-4)----------RMSD= 1.9000 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | -4.82 | -36.84 | -12.72 | 34.84 | -27.28 | 0.00 |
| CT | OS | P | OH | 3 | -2.57 | -46.67 | -17.30 | 44.08 | -20.64 | 0.00 |
| CT | OS | P | O2 | 3 | 27.60 | 40.78 | 20.00 | -80.00 | -46.48 | 0.00 |
| HC | CT | OS | P | 3 | 13.59 | -12.13 | 6.18 | 0.44 | 7.60 | 0.00 |
| HO | OH | P | O2 | 3 | 14.70 | -30.64 | -183.06 | 53.80 | 151.44 | 0.00 |
| HO | OH | P | OS | 3 | 12.48 | 45.86 | -134.28 | -34.48 | 95.44 | 0.00 |

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 SET6 (ORIG, Qopls, L-3)------------RMSD= 2.1710 kJ/mol
CT    OS     P     OS     3     2.47  -33.75  -17.36   31.28    0.00  0.00
CT    OS     P     OH     3     1.78  -50.38  -16.10   48.60    0.00  0.00
CT    OS     P     O2     3    40.00   40.00  -13.80  -80.00    0.00  0.00
HC    CT    OS     P      3    19.97  -20.09  -12.74    0.12    0.00  0.00
HO    OH     P     O2     3   -22.34  -25.54  -31.72   47.88    0.00  0.00
HO    OH     P     OS     3   -12.62   42.14  -40.00  -29.52    0.00  0.00

 SET7 (ORIG, Qopls, G-4)------------RMSD= 1.3890 kJ/mol
CT    OS     P     OS     3    25.73  -48.93  -13.74   13.56  -38.56  0.00
CT    OS     P     OH     3    25.29  -59.99   -2.14   23.40  -45.20  0.00
CT    OS     P     O2     3    45.35  -17.13   42.62  -46.60  -73.52  0.00
HC    CT    OS     P      3    55.44  -53.04    1.80    0.24   10.56  0.00
HO    OH     P     O2     3 -111.91  161.21  -89.48  -36.00   53.20  0.00
HO    OH     P     OS     3 -123.03  118.71  -88.64   13.40   36.32  0.00

 SET8 (ORIG, Qopls, G-3)------------RMSD= 1.4590 kJ/mol
CT    OS     P     OS     3    53.30  -41.18  -33.72  -12.12    0.00  0.00
CT    OS     P     OH     3    54.15  -57.03  -29.34    2.88    0.00  0.00
CT    OS     P     O2     3    67.47  -62.87  -21.22   -4.60    0.00  0.00
HC    CT    OS     P      3    37.38  -37.62    6.88    0.24    0.00  0.00
HO    OH     P     O2     3 -140.84  154.96  -38.38  -14.12    0.00  0.00
HO    OH     P     OS     3 -137.85  134.81  -55.08    3.04    0.00  0.00

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SET TYPE 3

 SET9  (M, Q0, L-3)----------------RMSD= 1.3550 kJ/mol
CT    OS     P     OS     3     7.99  -37.91  -40.00  29.92    0.00  0.00
CT    OS     P     OH     3     7.73  -49.93  -38.70  42.20    0.00  0.00
CT    OS     P     O2     3    39.29   37.87  -26.74 -77.16    0.00  0.00
HC    CT    OS     P      3    11.44  -11.72   16.96   0.28    0.00  0.00
HO    OH     P     O2     3   -18.63    3.79  -29.28  14.84    0.00  0.00
HO    OH     P     OS     3   -16.90   29.30  -39.86 -12.40    0.00  0.00

 SET10 (M, Q0, G-3)----------------RMSD= 1.1030 kJ/mol
CT    OS     P     OS     3    31.55  -20.75  -35.54  -10.80   0.00  0.00
CT    OS     P     OH     3    32.49  -32.13  -32.70   -0.36   0.00  0.00
CT    OS     P     O2     3    35.63  -34.43  -23.98   -1.20   0.00  0.00
HC    CT    OS     P      3    39.73  -39.21    3.34   -0.16   0.00  0.00
HO    OH     P     O2     3   -87.20  101.40  -39.12  -14.20   0.00  0.00
HO    OH     P     OS     3   -86.56   84.04  -55.72    2.52   0.00  0.00

 SET11 (M, Q0, L-4)----------------RMSD= 1.2780 kJ/mol
CT     OS     P     OS     3    5.43  -36.05  -27.12   27.40  -12.88  0.00
CT     OS     P     OH     3    7.19  -45.07  -27.78   35.24  -10.56  0.00
CT     OS     P     O2     3   31.08   31.16   -3.00  -68.12  -23.52  0.00
HC     CT    OS     P      3    0.48    3.82   21.52    0.32   18.48  0.00
HO     OH     P     O2     3   -4.90   -7.56  -98.78   29.68   68.88  0.00
HO     OH     P     OS     3   -3.66   35.50  -83.52  -20.92   43.68  0.00

 SET12 (M, Q0, G-4)----------------RMSD= 1.0600 kJ/mol
CT    OS     P     OS     3    14.01  -25.01   -23.06   4.36 -26.56  0.00
CT    OS     P     OH     3    13.67  -33.17   -14.78  11.60 -31.6   0.00
CT    OS     P     O2     3    20.37   -6.99    18.28 -25.84 -49.84  0.00
HC    CT    OS     P      3    54.23  -50.89    -8.94  -0.28  12.24  0.00
HO    OH     P     O2     3   -68.67  106.33   -74.38 -28.12  38.16  0.00
HO    OH     P     OS     3   -77.28   74.66   -77.92   9.16  26.16  0.00
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SET TYPE 4

SET13 (M, M, L-3)----------RMSD= 1.6160 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 5.63 | -37.79 | -35.80 | 32.16 | 0.00 | 0.00 |
| CT | OS | P | OH | 3 | 2.02 | -45.90 | -35.60 | 43.88 | 0.00 | 0.00 |
| CT | OS | P | O2 | 3 | 39.93 | 39.79 | -25.58 | -79.72 | 0.00 | 0.00 |
| HC | CT | OS | P | 3 | 19.95 | -20.15 | 1.92 | 0.20 | 0.00 | 0.00 |
| HO | OH | P | O2 | 3 | -16.14 | -2.86 | -29.38 | 19.00 | 0.00 | 0.00 |
| HO | OH | P | OS | 3 | -16.28 | 31.16 | -40.00 | -14.88 | 0.00 | 0.00 |

SET14 (M, M, G-3)----------RMSD= 1.2620 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 41.85 | -25.97 | -34.14 | -15.88 | 0.00 | 0.00 |
| CT | OS | P | OH | 3 | 39.50 | -33.82 | -31.86 | -5.68 | 0.00 | 0.00 |
| CT | OS | P | O2 | 3 | 46.18 | -53.66 | -23.64 | 7.48 | 0.00 | 0.00 |
| HC | CT | OS | P | 3 | 40.94 | -40.62 | -7.62 | -0.32 | 0.00 | 0.00 |
| HO | OH | P | O2 | 3 | -102.88 | 112.68 | -31.12 | -9.80 | 0.00 | 0.00 |
| HO | OH | P | OS | 3 | -101.91 | 101.31 | -45.42 | 0.60 | 0.00 | 0.00 |

SET15 (M, M, L-4)----------RMSD= 1.4680 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | -0.74 | -39.92 | -16.72 | 34.84 | -23.28 | 0.00 |
| CT | OS | P | OH | 3 | -1.47 | -43.97 | -19.74 | 40.56 | -19.52 | 0.00 |
| CT | OS | P | O2 | 3 | 29.40 | 39.40 | 14.22 | -79.20 | -41.6 | 0.00 |
| HC | CT | OS | P | 3 | 4.14 | 0.50 | 19.64 | 0.44 | 20.32 | 0.00 |
| HO | OH | P | O2 | 3 | 2.43 | -12.31 | -115.94 | 31.36 | 85.92 | 0.00 |
| HO | OH | P | OS | 3 | -0.85 | 36.69 | -94.24 | -22.28 | 54.24 | 0.00 |

SET16 (M, M, G-4)----------RMSD= 1.2170 kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | 19.90 | -31.33 | -18.44 | 3.72 | -30.88 | 0.00 |
| CT | OS | P | OH | 3 | 16.56 | -35.42 | -11.56 | 10.08 | -35.12 | 0.00 |
| CT | OS | P | O2 | 3 | 28.16 | -17.94 | 25.80 | -24.60 | -57.52 | 0.00 |
| HC | CT | OS | P | 3 | 56.96 | -52.64 | -20.72 | -0.48 | 15.36 | 0.00 |
| HO | OH | P | O2 | 3 | -79.10 | 116.18 | -72.16 | -26.20 | 43.52 | 0.00 |
| HO | OH | P | OS | 3 | -89.22 | 88.28 | -71.60 | 8.36 | 29.68 | 0.00 |

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The best RB parameters obtained from *fit_dihedral.py* program: for type set 1 (original vdW and Q0 charges) RMSD=2.623kJ/mol

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CT | OS | P | OS | 3 | -1.31 | -1.67 | -30.52 | 0.68 | -9.20 | 0.00 |
| CT | OS | P | OH | 3 | 2.75 | 1.93 | -30.36 | -6.60 | -7.68 | 0.00 |
| CT | OS | P | O2 | 3 | 3.72 | -4.02 | -27.88 | -0.44 | -2.96 | 0.00 |
| HC | CT | OS | P | 3 | 51.00 | -15.52 | -120.16 | -2.68 | 131.20 | 0.00 |
| HO | OH | P | O2 | 3 | 54.19 | 27.23 | -112.46 | -55.24 | 104.72 | 0.00 |
| HO | OH | P | OS | 3 | 17.88 | -27.46 | -72.46 | 27.48 | 71.60 | 0.00 |