**Supplementary Information**



**Supplementary Figure S1**: The block wise RMSD of the 6 duplex systems have shown here. First column is set-1 simulations. Second column is set-2 simulations. The a, b, c, d, e and f are the duplex systems. The 100 ns length simulation trajectory of each system has divided into four blocks (b1, b2, b3 and b4) of 25 ns each. The RMSD calculated for each block by considering the first frame of respective block as a reference structure.



**Supplementary Figure S2:** The average inter-strand phosphate distance along with standard deviations are given for (a) LNA-PS-LNA/RNA, (b) RcMOE-PS-RcMOE/RNA, (c) ScMOE-PS-ScMOE/RNA, (d) PS/RNA, (e) MOE-PS-MOE/RNA and (f) DNA/RNA duplexes, calculated for the 100 ns MD trajectory. Top plot showed set-1 simulations and bottom plot showed set-2 simulations.

**Supplementary Table S3:** The helical parameters X-displacement, inclination and h-twist were given for all the simulated duplexes along with the respective crystal structures. The three values are for start structure, after 50 ns and 100 ns structures respectively.

|  |  |  |  |
| --- | --- | --- | --- |
| **Duplex Systems** | **Average X-Displacement** | **Average Inclination** | **Average h-Twist** |
| **a** | -4.37 ± 4.77-7.43 ± 2.87-5.15 ± 4.61 | 11.44 ± 22.9524.62 ± 21.9010.69 ± 20.10 | 33.04 ± 12.1126.80 ± 7.9932.21 ± 13.89 |
| **b** | -2.98 ± 1.86-3.27 ± 2.37-4.69 ± 3.85 | 11.88 ± 15.4612.73 ± 8.9813.71 ± 16.88 | 30.25 ± 8.3132.15 ± 3.2328.16 ± 7.91 |
| **c** | -4.21 ± 1.31-3.97 ± 2.78-4.15 ± 2.16 | 13.21 *±* 14.9717.15 ± 19.089.79 ± 11.05 | 33.27 ± 7.7934.29 ± 10.5230.65 ± 5.96 |
| **d** | -5.00 ± 1.13-2.01 ± 2.14-4.44 ± 3.64 | 34.05 ± 10.927.83 ± 17.8622.57 ± 25.02 | 36.78 ± 2.941.66 ± 84.6039.63 ± 20.76 |
| **e** | -4.78 ± 1.64-5.30 ± 5.70-3.60 ± 2.59 | 20.31 ± 18.455.08 ± 10.883.49 ± 15.64 | 31.84 ± 7.9228.00 ± 8.3431.49 ± 5.07 |
| **1H0Q**  | -5.39 ± 1.17 | 11.55 ± 10.72 | 29.98 ± 2.99 |
| **8PSH**  | -3.56 ± 1.40 | 16.39 ± 10.19 | 35.08 ± 3.67 |
| **469D**  | -4.85 ± 0.82 | 23.83 ± 5.85 | 32.86 ± 2.69 |
| **2QKK**  | -3.36 ± 2.26 | 12.93 ± 16.22 | 32.08 ± 6.40 |

**Supplementary Table S4:** The base pair parameters shear, stretch, stagger, buckle, propeller and opening were given for all the six simulated duplexes.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Systems** | **Base Pair** | **Shear** | **Stretch** | **Stagger** | **Buckle** | **Propeller** | **Opening** |
| **a** | C-GT-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GT-A | 0.81 (1.1)0.01 (0.7)-0.21 (0.3)0.14 (0.7)-0.4 (0.4)0.40 (0.3)0.32 (0.2)0.63 (0.5)-0.09 (0.2)-0.47 (0.4)-0.59 (0.5)0.50 (0.3)-5.39 (0.9)0.47 (1.6) | 0.03 (0.6)0.17 (0.5)0.08 (0.2)0.07 (0.1)-0.18 (0.1)-0.22 (0.1)0.07 (0.1)-0.22 (0.1)0.07 (0.1)-0.12 (0.1)-0.21 (0.1)-0.18 (0.1)1.16 (0.1)-2.06 (0.2) | -0.24 (0.9)0.21 (0.5)-0.06 (0.5)-0.02 (0.5)0.02 (0.6)0.20 (0.6)0.01 (0.4)0.32 (0.5)0.08 (0.4)-0.20 (0.5)-0.15 (0.6)-0.24 (0.4)0.60 (1.0)-1.04 (2.4) | -25.85 (25)-17.77 (19)1.01 (16)-6.81 (14)-7.30 (12)-2.04 (14)-12.06 (13)-13.76 (11)-6.65 (11)1.95 (15)-0.51 (13)10.56 (14)10.02 (19)5.42 (44) | -5.90 (16)-12.81 (12)-17.34 (11)-9.53 (13)-19.52 (13)-11.66 (14)-11.47 (11)-7.20 (10)-6.25 (10)-8.85 (12)-19.27 (13)-1.56 (11)-17.60 (15)-0.52 (41) | 0.80 (16)-5.17 (10)-7.89 (6)-8.62 (6)-2.04 (6)-4.43 (4)-7.48 (5)-2.17 (7)-8.41 (5)-0.10 (5)-0.20 (7)-3.18 (4)32.74 (43)-11.94 (48)  |
| **b** | C-GU-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GU-A | 0.25 (1.7)-1.72 (2.4)-0.50 (3.4)0.25 (0.3)-0.11 (0.3)0.24 (0.3)0.16 (0.2)0.29 (0.2)-0.00 (0.2)-0.11 (0.3)-0.14 (0.3)0.19 (0.2)0.22 (0.3)0.12 (0.3) | -0.38 (2.9)-4.34 (5.0)-0.34 (0.1)0.09 (0.1)-0.03 (0.1)-0.08 (0.1)0.01 (0.1)-0.12 (0.1)-0.00 (0.1)-0.06 (0.1)-0.05 (0.1)-0.09 (0.1)-0.09 (0.1)-0.32 (1.1) | 0.62 (1.7)-0.48 (3.6)-0.97 (2.4)-0.62 (0.7)0.07 (0.4)-0.02 (0.3)-0.09 (0.4)0.02 (0.3)-0.05 (0.3)-0.04 (0.3)-0.00 (0.3)-0.00 (0.3)0.01 (0.3) -0.35 (2.2)  | -27.6 (76)-23.6 (47)-51.4 (29)-25.6 (17)6.42 (10)14.94 (10)8.73 (9)2.67 (9)4.25 (8)2.29 (8)4.02 (8)4.53 (8)3.19 (8)5.98 (79) | 10.0 (32)68.0 (41)-28.7 (51)2.10 (11)0.41 (9)-11.4 (7)-11.1 (7)-9.69 (7)-11.6 (7)-6.31 (7)-8.12 (7)-7.94 (7)-9.12 (7)2.26 (62) | -12.5 (55)94.07 (49)-4.44 (50)0.32 (7)0.026 (3)-0.63 (3)2.48 (6)-0.53 (3)2.19 (4)-0.36 (3)0.42 (3)-0.94 (3)-0.64 (3)-9.13 (68) |
| **c** | C-GU-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GU-A | 1.27 (3.2)1.70 (2.8)-0.85 (1.4)0.36 (0.6)-0.10 (0.3)0.25 (0.3)0.17 (0.2)0.29 (0.2)-0.00 (0.2)-0.13 (0.3)-0.14 (0.3)0.18 (0.2)0.27 (0.3)3.11 (7.2) | -5.49 (4.5)-4.61 (4.2)-1.06(1.5)0.11 (0.2)-0.02 (0.1)-0.08 (0.1)0.01 (0.1)-0.12 (0.1)-0.00 (0.1)-0.06 (0.1)-0.06 (0.1)-0.09 (0.1)-0.10 (0.1)-2.79 (5.5) | -4.90 (3.1)-4.34 (3.0)-2.34 (1.6)-0.41 (0.6)0.12 (0.4)-0.07 (0.3)-0.08 (0.4)0.01 (0.3)-0.07 (0.3)-0.03 (0.3)-0.02 (0.3)-0.03 (0.3)0.02 (0.3)3.20 (6.2) | -12.4 (57)5.36 (66)-28.7 (23)-24.5 (17)6.98 (10)15.77 (9)8.38 (9)3.12 (9)4.59 (8)2.73 (8)4.39 (8)4.59 (8)2.30 (8)22.60 (58) | -15.85 (41)-12.30 (24)-27.32 (18)8.13 (11)0.52 (9)-11.45 (7)-10.57 (7)-8.87 (7)-11.63 (7)-6.21 (7)-8.16 (7)-7.80 (7)-7.47 (7)-16.97 (35) | 34.4 (73)53.7 (47)-5.93 (17)2.79 (8)0.01 (3)-0.56 (3)2.66 (6)-0.64 (3)2.37 (4)-0.07 (3)0.39 (3)-0.62 (3)-0.98 (3)-18.5 (71) |
| **d** | C-GU-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GU-A | 1.09 (1.3)1.64 (4.2)-2.40 (3.9)1.87 (6.8)-0.13 (0.7)0.44 (0.3)0.21 (0.6)0.59 (0.3)-0.13 (0.2)-0.84 (1.2)-1.33 (1.5)1.42 (1.5)-5.67 (4.4)-3.13 (4.9) | -3.27 (3.7)0.49 (1.6)-1.56 (4.5)-0.62 (2.9)0.33 (0.5)-0.21 (0.1)0.05 (0.1)-0.25 (0.1)0.08 (0.1)-0.01 (0.4)0.32 (1.0)0.06 (0.4)-2.84 (3.1)1.04 (4.6) | -1.62 (2.5)0.12 (3.8)-3.69 (4.5)-0.37 (4.4)-0.61 (0.7)0.51 () 0.6 0.09 (0.5)0.26 (0.4)-0.09 (0.4)-0.03 (0.6)0.40 (0.9)0.04 (0.9)-0.36 (3.6)-5.55 (6.2) | -3.86 (38)-1.10 (30)18.19 (24)-36.81 (89)-49.85 (31)-13.06 (18)-5.62 (13)-4.33 (11)6.96 (12)-2.44 (13)-2.51 (16)12.66 (25)-79.73 (65)-31.69 (77) | -2.30 (32)10.95 (34)-26.40 (49)-7.88 (32)-13.45 (14)-9.81 (12)-11.48 (11)-4.86 (10)-14.32 (10)-12.61 (11)-23.57 (14)-17.17 (13)-16.10 (28)21.58 (50) | -14.57 (27)-5.54 (72)-31.81 (75)-7.46 (102)-2.64 (11)-4.45 (4)-6.95 (6)-3.99 (4)-7.56 (5)4.55 (20)14.69 (30)12.42 (24)-33.27 (56)-49.75 (95) |
| **e** | C-GU-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GU-A | 0.32 (1.3)2.54 (2.1)0.19 (0.8)0.18 (0.3)-0.09 (0.3)0.25 (0.3)0.18 (0.2)0.29 (0.2)-0.01 (0.2)-0.11 (0.3)-0.13 (0.3)0.19 (0.2)0.30 (0.3)0.61 (4.5) | -0.12 (2.1)-5.45 (4.4)-0.13 (0.9)0.07 (0.1) -0.03 (0.1)-0.09 (0.1)0.01 (0.1)-0.12 (0.1)-0.00 (0.1)-0.06 (0.1)-0.05 (0.1)-0.08 (0.1)-0.11 (0.1)-0.73 (4.9) | 0.15 (1.6)-4.36 (3.0)-0.51 (0.9)-0.51 (0.7)0.11 (0.4)3.73 (0.3)-0.07 (0.4)0.02 (0.3)-0.01 (0.3)-0.01 (0.3)0.04 (0.3)-0.08 (0.3)-0.07 (0.3)0.09 (2.9) | 12.8 (16)-30.1 (29)-37.5 (28)-23.0 (20)4.99 (11)13.8 (9)8.67 (9)3.16 (9)4.88 (9)3.21 (8)6.47 (9)9.37 (8)4.79 (8)0.08 (34) | -14.0 (14)-5.22 (25)-28.5 (13)-1.30 (11)-1.91 (9)-11.2 (7)-9.58 (8)-9.40 (8)-9.86 (7)-5.46 (7)-5.77 (7)-7.51 (8)-13.3 (8)-5.62 (27) | 2.65 (19)3.52 (44)8.85 (15) 2.96 (6.6)-0.06 (3.2)-1.04 (3.2)1.74 (5.7)-0.60 (3.1)1.75 (4.8)-0.69 (3.1)0.00 (3.1)-0.78 (3.0)-0.03 (3.3)-1.67 (52) |
| **f** | C-GU-AT-AA-TG-CC-GA-TC-GT-AG-CG-CC-GC-GU-A | 4.01 (4.5)0.01 (0.6)0.17 (0.3)-0.08 (0.3)0.21 (0.3)0.15 (0.2)0.21 (0.3)-0.01 (0.2)-0.09 (0.3)-0.11 (0.3)0.18 (0.3)0.24 (0.3)0.50 (0.7) | -2.35 (3.4)-0.85 (2.0)0.03 (0.1)-0.01 (0.1)-0.04 (0.1)0.02 (0.1)-0.07 (0.1)0.01 (0.1)-0.05 (0.1)-0.04 (0.1)-0.05 (0.1)-0.08 (0.1)-0.17 (0.8) | -2.88 (3.1)-1.44 (2.3)-0.56 (0.6)0.28 (0.4)-0.05 (0.3)-0.10 (0.4)-0.00 (0.3)0.00 (0.4)-0.01 (0.3)0.06 (0.3)-0.16 (0.3)-0.01 (0.3)0.06 (0.5) | -50.9 (38)-29.6 (33)-12.4 (16)12.61 (11)17.1 (9)7.19 (9)4.41 (9)3.92 (10)3.71 (9)7.31 (10)10.40 (9)2.84 (8)1.26 (13) | 54.8 (71)-18.4 (11)-2.29 (9)-6.64 (8)-15.6 (7)-11.8 (8)-10.6 (8)-12.8 (8)-5.76 (8)-7.66 (8)-10.6 (7)-9.10 (8)-12.1 (11) | 5.19 (40)9.82 (14)-0.11 (6.2)-0.33 (3.3)0.21 (3.7)1.32 (6.7)-0.10 (3.7)1.84 (6.4)-0.52 (3.4)0.00 ()3.3 0.11 (3.2)-0.13 (3.1)-2.14 (9.2) |

**Supplementary Table S5:** The base pair parameters shear, stretch, stagger, buckle, propeller and opening were given for all the six simulated duplexes.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Systems** | **Base Pair** | **Shift** | **Slide** | **Rise**  | **Tilt** |  **Roll** | **Twist** |
| **a** | C-G/ T-AT-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ T-A | -0.10 (1.0)-0.02 (0.7)0.02 (0.6)0.44 (0.8)-0.19 (0.7)-0.59 (0.7)0.39 (0.6)-0.07 (0.6)-0.03 (0.5)1.35 (1.2)-0.29 (0.7)1.04 (2.1)-0.81 (2.1) | -2.30 (0.9)-1.96 (0.6)-1.55 (0.6)-1.79 (0.6)-1.79 (0.9)-1.22 (0.6)-0.70 (0.9)-1.09 (0.4)-0.37 (0.6)-1.33 (0.9)-1.96 (1.1)-2.10 (0.5)-1.46 (1.8) | 3.35 (0.5)3.06 (0.6)3.57 (0.5)3.43 (0.4)3.26 (0.3)3.60 (0.6)3.45 (0.3)3.22 (0.3)3.27 (0.4)3.44 (0.5)3.23 (0.4)3.57 (0.5)4.21 (1.8) | -0.6 (7.3)2.22 (5.8)-1.2 (6.1)0.49 (6.4)-0.4 (7.2)1.84 (5.8)1.14 (5.5)2.66 (4.9)0.16 (5.3)-1.8 (7.0)-2.0 (7.3)-5.1 (6.8)0.28 (15) | 8.81 (8.1)10.2 (10)10.9 (9.4)7.47 (9.1)4.89 (7.0)4.05 (9.5)-0.12 (6.9)0.62 (6.7)9.99 (7.2)12.1 (9.4)9.38 (9.2)4.53 (10)-7.57 (25) | 18.9 (7.2)22.6 (6.8)28.3 (6.1)27.1 (5.9)35.5 (4.7)30.1 (4.4)35.7 (4.2)31.2 (4.3)7.42 (9.9)19.9 (9.3)33.6 (5.4)20.5 (10)35.3 (22) |
| **b** | C-G/ U-AU-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ U-A | 3.68 (2.7)4.39 (2.4)0.49 (1.9)0.65 (0.8)-0.4 (0.5)0.09 (0.6)-0.3 (0.5)-0.0 (0.6)-0.0 (0.5)0.09 (0.6)-0.1 (0.4)-0.2 (0.4)1.20 (1.1) | 0.53 (3.7)2.70 (2.0)1.18 (1.3)-0.77 (1.1)-1.13 (0.7)-1.40 (0.4)-1.82 (0.5)-1.72 (0.4)-1.33 (0.4)-2.02 (0.4)-1.94 (0.5)-2.05 (0.3)-2.00 (0.5) | 3.31 (1.8)2.37 (1.5)3.54 (1.4)2.74 (0.3)3.24 (0.2)3.50 (0.4)3.49 (0.2)3.34 (0.3)3.37 (0.3)3.28 (0.3)3.36 (0.2)3.36 (0.3)3.26 (0.6) | -9.48 (33)11.9 (26)-11.0 (16)-6.62 (8.0)-1.74 (4.3)-3.02 (4.8)-4.15 (4.4)0.03 (4.0)-2.87 (4.3)-3.31 (4.4)-2.63 (4.1)-1.68 (4.4)9.99 (30) | -34.4 (22)79.2 (44)7.74 (21)4.81 (6.9)2.49 (5.2)8.97 (6.6)3.88 (5.0)2.43 (4.9)9.71 (6.3)5.97 (5.4)1.40 (4.5)3.86 (5.3)-7.11 (42) | -21.7 (36)87.59 (51)27.29 (27)17.18 (7.4)33.41 (4.0)30.77 (3.7)30.70 (3.8)27.76 (4.4)29.98 (3.9)25.62 (4.6)31.76 (4.0)28.46 (4.6)32.24 (34) |
| **c** | C-G/ U-AU-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ U-A | 1.58 (1.7)-0.30 (2.2)1.04 (1.1)0.70 (0.8)-0.40 (0.4)0.08 (0.6)-0.34 (0.5)-0.03 (0.5)-0.04 (0.5)0.15 (0.6)-0.13 (0.4)-0.14 (0.4)-0.70 (0.4) | 1.55 (1.7)1.76 (1.9)0.77 (1.2)-1.26 (0.7)-1.24 (0.6)-1.47 (0.4)-1.88 (0.5)-1.79 (0.4)-1.31 (0.5)-1.99 (0.4)-1.97 (0.5)-2.09 (0.3)-3.67 (2.1) | 2.41 (1.6)4.45 (1.4)4.03 (0.8)2.79 (0.3)3.24 (0.2)3.52 (0.4)3.47 (0.2)3.33 (0.3)3.37 (0.3)3.28 (0.3)3.36 (0.2)3.39 (0.3)0.93 (3.7) | -0.43 (36)-40.4 (35)-18.7 (13)-3.03 (7.3)-0.91 (4.5)-3.54 (4.9)-4.01 (4.4)0.14 (4.1)-3.23 (4.4)-3.06 (4.3)-2.57 (4.1)-1.92 (4.3)-8.04 (28) | 9.95 (21)2.94 (19)18.3 (9.5)4.95 (7.0)2.01 (5.6)8.83 (6.7)3.69 (4.9)2.66 (5.0)10.3 (6.6)6.36 (5.5)1.69 (4.5)3.97 (5.4)1.03 (22) | -2.85 (41)-14.6 (32)31.23 (10)14.36 (7.1)33.71 (4.2)30.48 (3.7)30.32 (4.2)27.98 (3.6)29.57 (4.0)25.79 (5.0)31.46 (4.1)29.15 (4.3)41.09 (37) |
| **d** | C-G/ U-AU-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ U-A | 0.20 (2.0)-0.78 (2.2)1.57 (4.5)1.45 (2.0)-0.11 (0.7)-0.32 (0.6)0.25 (0.7)-0.61 (0.6)0.44 (1.1)0.93 (1.1)-0.11 (0.8)0.78 (1.3)0.79 (2.2) | -0.56 (2.0)-1.40 (1.7)-2.70 (3.1)0.96 (1.6)-0.78 (0.9)-0.88 (0.6)-1.26 (1.0)-1.51 (0.4)-1.22 (0.7)-1.53 (0.7)-0.52 (1.4)-1.55 (1.2)0.46 (1.8) | 4.13 (2.2)2.08 (2.2)5.41 (2.4)3.27 (1.0)2.84 (0.3)3.17 (0.5)3.38 (0.3)3.13 (0.4)3.61 (0.5)3.21 (0.5)3.15 (0.5)2.96 (1.3)-0.28 (2.3) | -13.8 (30)0.99 (20)-10.1 (33)4.23 (31)-7.92 (8.3)1.84 (5.7)-0.58 (6.2)0.66 (5.1)-3.71 (5.6)-1.59 (7.4)1.85 (8.1)-63.9 (50)-0.08 (37) | 19.8 (39)-6.60 (27)12.1 (43)1.46 (21)10.0 (7.8)5.50 (8.1)2.97 (8.0)4.40 (6.2)9.48 (8.2)10.7 (8.0)6.90 (7.7)43.2 (37)18.0 (36) | 24.32 (35)4.77 (49)44.16 (78)20.49 (59)28.74 (6.4)27.66 (5.3)34.31 (5.2)24.53 (4.6)21.94 (8.2)25.82 (7.8)41.05 (11)-43.5 (62)-7.43 (58) |
| **e** | C-G/ U-AU-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ U-A | -0.47 (2.5)1.52 (1.9)0.31 (0.7)0.31 (0.9)-0.25 (0.5)0.10 (0.6)-0.37 (0.5)0.01 (0.5)-0.09 (0.5)-0.15 (0.6)-0.19 (0.4)-0.45 (0.5)-0.15 (2.8) | 0.45 (2.0)2.14 (2.3)0.89 (1.6)-0.54 (1.2)-1.12 (0.7)-1.38 (0.5)-1.82 (0.5)-1.71 (0.4)-1.42 (0.5)-2.02 (0.5)-1.87 (0.5)-1.83 (0.3)-2.19 (1.4) | 6.57 (1.8)5.62 (2.0)3.24 (0.4)2.79 (0.4)3.23 (0.2)3.51 (0.4)3.51 (0.2)3.37 (0.3)3.40 (0.3)3.26 (0.3)3.35 (0.2)3.45 (0.3)3.28 (1.4) | 22.9 (14)-16.0 (18)-10.3 (8.5)-6.55 (8.0)-1.36 (4.4)-3.02 (4.8)-4.13 (4.4)-0.63 (4.1)-2.87 (4.5)-3.98 (4.5)-2.51 (4.1)-2.77 (4.8)0.41 (16) | 12.2 (12)-2.22 (21)17.3 (9.7)5.48 (6.3)1.73 (5.0)6.59 (6.5)2.34 (5.0)0.44 (5.0)6.33 (6.5)4.41 (5.4)0.58 (4.7)3.90 (5.3)9.14 (15) | 45.8 (18)-3.58 (17)26.6 (8.6)20.4 (8.7)33.2 (4.0)31.4 (3.9)30.4 (4.6)28.6 (3.5)30.4 (4.2)26.5 (4.7)30.6 (4.6)32.3 (4.0)31.8 (29) |
| **f** | C-G/ U-AU-A/ T-AT-A/ A-TA-T/ G-CG-C/ C-GC-G/ A-TA-T/ C-GC-G/ T-AT-A/ G-CG-C/ G-CG-C/ C-GC-G/ C-GC-G/ U-A | 0.07 (1.9)0.35 (0.8)-0.27 (0.8)0.05 (0.5)-0.09 (0.7)-0.14 (0.7)0.06 (0.6)-0.29 (0.8)-0.17 (0.7)-0.12 (0.5)-0.16 (0.5)-0.12 (0.6) | 0.75 (1.9)1.90 (1.3)0.19 (0.9)-1.21 (0.5)-1.45 (0.4)-1.68 (0.6)-1.65 (0.4)-1.29 (0.5)-1.61 (0.6)-1.58 (0.5)-1.86 (0.4)-1.58 (0.4) | 5.46 (2.4)3.55 (1.2)2.83 (0.4)3.28 (0.2)3.57 (0.4)3.41 (0.2)3.40 (0.3)3.35 (0.4)3.23 (0.3)3.30 (0.2)3.51 (0.3)3.45 (0.3) | 3.43 (23)-15.0 (14)-9.69 (6.1)-0.84 (4.4)-3.33 (4.9)-3.37 (4.4)-0.18 (4.3)-3.06 (4.7)-3.64 (4.5)-1.20 (4.1)-3.31 (4.3)-0.76 (4.9) | -20.2 (31)12.8 (8.1)3.86 (6.6)2.81 (5.1)11.0 (7.2)4.42 (5.4)3.08 (5.2)9.76 (6.6)5.77 (5.4)2.25 (4.7)6.47 (5.0)2.45 (6.1) | -2.38 (28)19.21 (9.2)27.92 (5.7)33.00 (4.3)29.61 (4.9)29.16 (4.8)29.23 (4.5)26.08 (8.3)28.06 (5.5)31.82 (4.4)29.97 (4.1)31.93 (8.7) |

**Supplementary Table S6:** The base pair hydrogen bonds along with their residence time have showed here for all the duplexes.

|  |
| --- |
| **Set - 1** |
| **Base Pair** | **H-Bond** | **System** **(a)** | **System****(b)** | **System****(c)** | **System****(d)** | **System****(e)** | **System****(f)** |
| **1C:G28** | **N3---H1-N1****N4-H42---O6****N4-H41---O4****O2---H21-N2****O2---H22-N2****N4-H41---O6****O2---H1-N1** | 82.4544.4343.4442.9441.12------ | 60.08------60.41---59.44--- | --------------------- | 52.10------------------ | ---------89.98------56.43 | --------------------- |
| **2T:A27** | **N3-H3---N1****O4---H61-N6****O4---H62-N6****N3-H3---N7** | 94.6247.2243.34--- | ------51.9055.01 | ------------ | 53.17--------- | ------------ | ------------ |
| **3T:A26** | **N3-H3---N1****O4---H62-N6****O4---H61-N6** | 98.0646.7143.17 | 71.33---64.96 | --------- | 52.47------ | 87.26---76.71 | 76.64---58.51 |
| **3T:A27** | **O2---H61-N6****N3-H3---N1****O4---H61-N6** | --------- | 69.24------ | ---62.1553.95 | --------- | --------- | --------- |
| **3T:G28** | **O2---H1-N1** | --- | --- | 48.76 | --- | --- | --- |
| **4A:U25** | **N1---H3-N3****N6-H62---O4****N6-H61---O4** | 96.9946.4545.61 | 91.88---96.56 | 95.43---94.43 | --------- | 94.26---95.91 | 97.33---97.89 |
| **5G:C24** | **N1-H1---N3****N2-H22---O2****N2-H21---O2****O6---H41-N4****O6---H42-N4** | 98.1750.6647.8946.3346.18 | 99.99---99.9999.15--- | 99.89---99.9099.02--- | 74.9045.6740.69------ | 99.97---99.9499.30--- | 99.93---99.8098.73--- |
| **6C:G23** | **N3---H1-N1****O2---H21-N2****N4-H41---O6****O2---H22-N2****O2---H1-N1** | 99.4551.7648.3246.88--- | 99.9599.9999.64------ | 99.9899.9999.58---40.20  | 99.3244.6344.5753.4044.03 | 99.9799.9799.65---40.89 | 99.9099.9999.04------ |
| **7A:U22** | **N1---H3-N3****N6-H62---O4****N6-H61---O4** | 99.5347.9845.82 | 99.79---96.52 | 99.82---96.20 | 98.0041.9448.55 | 99.88---96.95 | 99.65---95.36 |
| **8C:G21** | **N3---H1-N1****O2---H1-N1****O2---H22-N2****N4-H41---O6****O2---H21-N2** | 97.7960.8550.9048.0045.63 | 100.0047.27---99.5499.99 | 99.9847.93---99.61100.00 | 99.5454.9948.1446.8149.50 | 99.9948.13---99.6699.99 | 99.74------99.2699.96 |
| **9T:A20** | **N3-H3---N1****O4---H62-N6****O4---H61-N6** | 99.1047.9647.89 | 99.95---98.02 | 99.97---98.08 | 99.2949.0346.26 | 100.00---98.44 | 99.68---94.86 |
| **10G:C19** | **N1-H1---N3****N2-H22---O2****O6---H42-N4****O6---H41-N4****N2-H21---O2** | 97.4550.2147.1747.1047.03 | 99.97------99.7099.98 | 99.90------99.5699.98 | 85.2746.62---42.5143.39 | 99.97------99.5899.97 | 99.87------99.3799.94 |
| **11G:C18** | **N1-H1---N3****N2-H22---O2****N2-H21---O2****O6---H41-N4****O6---H42-N4** | 95.6050.0645.8645.4644.24 | 99.96---99.9999.38--- | 99.93---100.0099.49--- | 72.7142.5645.92------ | 99.96---99.9999.39--- | 99.91---99.9799.06--- |
| **12C:G17** | **N3---H1-N1****O2---H21-N2****N4-H41---O6****O2---H22-N2****O2---H1-N1** | 99.6651.7451.1447.0744.43 | 99.9999.9999.76------ | 99.9999.9899.71------ | 76.76------41.7259.68 | 99.99100.0099.47------ | 99.99100.0099.50------ |
| **13C:G16** | **N3---H1-N1****O2---H21-N2****O2---H22-N2****N4-H41---O6****O2---H1-N1** | 59.8349.7441.37------ | 100.00100.00---99.75--- | ---99.98------40.69 | --------------- | 100.00------47.30 | 99.9999.98---99.59--- |
| **14T:A15** | **N3-H3---N1****O4---H61-N6** | ------ | 53.1250.90 | ------ | ------ | ---75.80 | 87.3784.46 |
| **14T:G17** | **N3-H3---N3** | --- | --- | --- | 57.80 | --- | --- |
| **Set - 2** |
| **Base Pair** | **H-Bond** | System (a) | System(b) | System(c) | System(d) | System(e) | System(f) |
| **1C:G28** | **N3---H1-N1****N4-H42---O6****N4-H41---O4****O2---H21-N2****O2---H22-N2****N4-H41---O6****O2---H1-N1** | 45.66------------------ | --------------------- | ---------99.75------44.93 | 95.50------45.8544.7547.2446.59 | --------------------- | --------------------- |
| **2T:A27** | **N3-H3---N1****O4---H61-N6****O4---H62-N6****N3-H3---N7** | 51.11--------- | ------------ | ------69.75--- | 96.1941.4640.84--- | ---48.85------ | ------------ |
| **2T:G28** | **O2---H1-N1** | --- | --- | --- | --- | 52.94 | --- |
| **3T:A26** | **N3-H3---N1****O4---H62-N6****O4---H61-N6** | 96.3840.8444.49 | --------- | 92.39---86.84 | 95.1143.0346.28 | 97.70---97.03 | 76.64---58.51 |
| **3T:A27** | **O2---H61-N6****N3-H3---N1****O4---H61-N6** | --------- | --------- | 63.95------ | --------- | --------- | --------- |
| **3T:G28** | **O2---H1-N1** | --- | --- | --- | --- | --- | --- |
| **4A:U25** | **N1---H3-N3****N6-H62---O4****N6-H61---O4** | 96.4345.8047.26 | 51.48---62.83 | 98.20---94.98 | 55.43------ | 99.93---95.57 | 97.33---97.89 |
| **5G:C24** | **N1-H1---N3****N2-H22---O2****N2-H21---O2****O6---H41-N4****O6---H42-N4** | 97.2348.9349.5149.1142.93 | 99.77---99.9297.41--- | 99.90---99.9098.59--- | 87.2547.7142.1242.6742.72 | 99.94---99.9898.74 | 99.93---99.8098.73--- |
| **6C:G23** | **N3---H1-N1****O2---H21-N2****N4-H41---O6****O2---H22-N2****O2---H1-N1** | 99.5648.4147.9849.7940.03 | 99.9799.9399.65--- | 99.9599.9999.49---40.89 | 99.5045.5247.5651.0154.27 | 99.9899.9999.60------ | 99.9099.9999.04------ |
| **7A:U22** | **N1---H3-N3****N6-H62---O4****N6-H61---O4** | 99.5442.0153.43 | 99.70---95.34 | 99.75---96.60 | --------- | 99.83---96.92 | 99.65---95.36 |
| **8C:G21** | **N3---H1-N1****O2---H1-N1****O2---H22-N2****N4-H41---O6****O2---H21-N2** | 99.1350.5547.4148.5650.64 | 99.9149.55---99.5899.98 | 99.9948.19---99.68100.00 | 92.5748.4049.7141.62--- | 99.9846.51---99.6099.99 | 99.74------99.2699.96 |
| **9T:A20** | **N3-H3---N1****O4---H62-N6****O4---H61-N6** | 99.5346.1147.13 | 99.98---97.16 | 99.97---97.23 | 94.3446.5540.61 | 99.94---97.88 | 99.68---94.86 |
| **10G:C19** | **N1-H1---N3****N2-H22---O2****O6---H42-N4****O6---H41-N4****N2-H21---O2** | 97.2849.3446.4946.9245.87 | 99.97------99.6099.99 | 99.74------99.50100.00 | 68.6041.28------41.30 | 99.79------99.4899.99 | 99.87------99.3799.94 |
| **11G:C18** | **N1-H1---N3****N2-H22---O2****N2-H21---O2****O6---H41-N4****O6---H42-N4** | 89.4348.6647.1541.0141.94 | 99.82---99.9899.22--- | 99.86---99.9999.24--- | --------------- | 99.98---100.0099.41--- | 99.91---99.9799.06--- |
| **12C:G17** | **N3---H1-N1****O2---H21-N2****N4-H41---O6****O2---H22-N2****O2---H1-N1** | 99.7050.8249.3648.1640.09 | 99.9699.9999.65------ | 100.00100.0099.73------ | 83.1241.4946.8343.0351.27 | 99.93100.0099.44------ | 99.99100.0099.50------ |
| **13C:G16** | **N3---H1-N1****O2---H21-N2****O2---H22-N2****N4-H41---O6****N4-H42---O6****O2---H1-N1** | 98.7952.4545.9149.1747.8941.30 | 100.0099.97---99.81---42.38 | ---99.94------------ | 46.8999.85---------49.47 | ------------------ | 99.9999.98---99.59------ |
| **14T:A15** | **N3-H3---N1****O4---H61-N6****O2---H62-N6** | 60.69------ | ------63.23 | --------- | --------- | --------- | 87.3784.46--- |
| **14T:G17** | **N3-H3---N3** | --- | --- | --- | --- | --- | --- |

**Supplementary Data: FRCMOD files and PREPI files as Supplementary as recommended by Referees.**

FRCMOD files

frcmod.ADS:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

HC 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

CB 12.010 0.360 same as c2

CA 12.010 0.360 same as c2

NC 14.010 0.530 same as n2

CQ 12.010 0.360 same as c2

H5 1.008 0.135 same as ha

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

NB 14.010 0.530 same as n2

CK 12.010 0.360 same as c2

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

CT-HC 337.30 1.092 same as c3-hc

N\*-CB 411.10 1.391 same as c2-na

N\*-CK 411.10 1.391 same as c2-na

CB-CB 418.30 1.429 same as cc-cc

CB-NC 431.60 1.376 same as cc-nc

CB-CA 411.70 1.434 same as ca-cc

CB-NB 431.60 1.376 same as cc-nc

CA-NC 492.90 1.336 same as ca-nc

CA-N2 449.00 1.364 same as ca-nh

NC-CQ 431.60 1.376 same as cc-nc

CQ-H5 344.30 1.087 same as c2-ha

N2-H 394.10 1.018 same as hn-n3

NB-CK 431.60 1.376 same as cc-nc

CK-H5 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-H1 46.400 110.050 same as c3-c3-hc

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-CT-HC 46.400 110.050 same as c3-c3-hc

CT-N\*-CB 64.200 117.200 same as c2-na-c3

CT-N\*-CK 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

HC-CT-HC 39.400 108.350 same as hc-c3-hc

N\*-CB-CB 69.800 121.380 same as c2-c2-na

N\*-CB-NC 71.700 123.620 same as n2-c2-na

N\*-CK-NB 71.700 123.620 same as n2-c2-na

N\*-CK-H5 51.200 112.420 same as ha-c2-na

CB-N\*-CK 67.800 110.370 same as c2-na-c2

CB-CB-CA 67.700 111.040 same as ca-cc-cc

CB-CB-NB 70.000 113.420 same as cc-cc-nc

CB-NC-CQ 68.600 110.190 same as cc-nc-cc

CB-CB-NC 70.000 113.420 same as cc-cc-nc

CB-CA-NC 70.000 113.420 same as cc-cc-nc

CB-CA-N2 68.600 118.980 same as cc-cc-nh

CB-NB-CK 68.600 110.190 same as cc-nc-cc

CA-CB-NB 70.000 113.420 same as cc-cc-nc

CA-NC-CQ 69.426 110.070 Calculated with empirical approach

CA-NC-CQ 68.600 110.190 same as cc-nc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

NC-CA-N2 72.800 118.860 same as nc-ca-nh

NC-CQ-H5 52.400 120.540 same as ha-c2-n2

NC-CQ-NC 68.100 123.870 same as ne-ce-ne

H -N2-H 41.300 107.130 same as hn-n3-hn

NB-CK-H5 52.400 120.540 same as ha-c2-n2

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-H1 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-OS-CT 1 0.383 0.000 3.000 same as X -c3-os-X

OS-CT-CT-HC 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-N\*-CB 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CB 1 2.500 0.000 1.000 same as os-c3-na-c2

OS-CT-N\*-CK 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CK 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-CB-CB 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CB-NC 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CK-NB 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CK-H5 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-CB 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CK 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CB 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CK 1 0.000 0.000 2.000 same as X -c3-na-X

HC-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

HC-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CB-CB-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CB-CB-NB 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CB-NC-CQ 1 4.150 180.000 2.000 same as X -c2-n2-X

N\*-CK-NB-CB 1 4.150 180.000 2.000 same as X -c2-n2-X

CB-N\*-CK-NB 1 0.625 180.000 2.000 same as X -c2-na-X

CB-N\*-CK-H5 1 0.625 180.000 2.000 same as X -c2-na-X

CB-CB-CA-NC 1 4.000 180.000 2.000 same as X -cc-cc-X

CB-CB-CA-N2 1 4.000 180.000 2.000 same as X -cc-cc-X

CB-CB-NB-CK 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-NC-CQ-NC 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-NC-CQ-H5 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-CB-N\*-CK 1 0.625 180.000 2.000 same as X -c2-na-X

CB-CB-NC-CQ 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-CA-NC-CQ 1 4.800 180.000 2.000 same as X -ca-nc-X

CB-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CB-NB-CK-H5 1 4.750 180.000 2.000 same as X -cc-nc-X

CA-CB-CB-NC 1 4.000 180.000 2.000 same as X -cc-cc-X

CA-CB-NB-CK 1 4.750 180.000 2.000 same as X -cc-nc-X

CA-NC-CQ-H5 1 4.750 180.000 2.000 same as X -cc-nc-X

CA-NC-CQ-NC 1 4.750 180.000 2.000 same as X -cc-nc-X

NC-CA-CB-NB 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CQ-NC-CA-N2 1 4.800 180.000 2.000 same as X -ca-nc-X

N2-CA-CB-NB 1 4.000 180.000 2.000 same as X -cc-cc-X

NB-CB-CB-NC 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CB-N\*-CK 1 0.625 180.000 2.000 same as X -c2-na-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 HC 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 CB 1.9080 0.0860 same as cc

 CA 1.9080 0.0860 same as ca

 NC 1.8240 0.1700 same as nc

 CQ 1.9080 0.0860 same as cc

 H5 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 NB 1.8240 0.1700 same as nc

 CK 1.9080 0.0860 same as cc

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frcmod.TDS:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

HC 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CM 12.010 0.360 same as c2

H4 1.008 0.135 same as ha

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

CT-HC 337.30 1.092 same as c3-hc

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

C -CM 449.90 1.406 same as c -c2

CM-CT 328.30 1.508 same as c2-c3

CM-CM 418.30 1.429 same as cc-cc

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-H1 46.400 110.050 same as c3-c3-hc

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-CT-HC 46.400 110.050 same as c3-c3-hc

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

HC-CT-HC 39.400 108.350 same as hc-c3-hc

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NA 73.200 115.400 same as na-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-C 64.700 126.400 same as c -na-c

O -C -NA 75.000 122.850 same as na-c -o

NA-C -CM 0.000 0.000 ATTN, need revision

C -CM-CT 63.900 119.700 same as c -c2-c3

C -CM-CM 67.900 120.700 same as c -c2-c2

O -C -CM 72.800 119.120 same as c2-c -o

CM-CT-HC 47.000 110.490 same as c2-c3-hc

CM-CM-H4 50.000 120.940 same as c2-c2-ha

CT-CM-CM 64.300 123.420 same as c2-c2-c3

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-H1 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-OS-CT 1 0.383 0.000 3.000 same as X -c3-os-X

OS-CT-CT-HC 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NA 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NA 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

HC-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

HC-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

N\*-C -NA-C 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-C 1 0.350 180.000 4.000 same as X -c -na-X

N\*-CM-CM-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-CT 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -O 1 0.350 180.000 4.000 same as X -c -na-X

C -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NA-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CM-CT 1 2.175 180.000 2.000 same as X -c -c2-X

NA-C -CM-CM 1 2.175 180.000 2.000 same as X -c -c2-X

H -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

H -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

C -CM-CT-HC 1 0.000 0.000 2.000 same as X -c2-c3-X

C -CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

O -C -CM-CT 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -CM-CM 1 2.175 180.000 -2.000 same as c2-c2-c -o

O -C -CM-CM 1 0.300 0.000 3.000 same as c2-c2-c -o

CT-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

HC-CT-CM-CM 1 0.380 180.000 -3.000 same as hc-c3-c2-c2

HC-CT-CM-CM 1 1.150 0.000 1.000 same as hc-c3-c2-c2

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 HC 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CM 1.9080 0.0860 same as cc

 H4 1.4870 0.0157 same as hc

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frcmod.GDS:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

HC 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

CB 12.010 0.360 same as c2

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CA 12.010 0.360 same as c2

N2 14.010 0.530 same as n3

NB 14.010 0.530 same as n2

NC 14.010 0.530 same as n2

CK 12.010 0.360 same as c2

H5 1.008 0.135 same as ha

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

CT-HC 337.30 1.092 same as c3-hc

N\*-CB 411.10 1.391 same as c2-na

N\*-CK 411.10 1.391 same as c2-na

CB-CB 418.30 1.429 same as cc-cc

CB-NC 431.60 1.376 same as cc-nc

CB-C 449.90 1.406 same as c -c2

CB-NB 431.60 1.376 same as cc-nc

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

NA-CA 411.10 1.391 same as c2-na

CA-N2 449.00 1.364 same as ca-nh

CA-NC 492.90 1.336 same as ca-nc

N2-H 394.10 1.018 same as hn-n3

NB-CK 431.60 1.376 same as cc-nc

CK-H5 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-CT-HC 46.400 110.050 same as c3-c3-hc

CT-N\*-CB 64.200 117.200 same as c2-na-c3

CT-N\*-CK 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

HC-CT-HC 39.400 108.350 same as hc-c3-hc

N\*-CB-CB 69.800 121.380 same as c2-c2-na

N\*-CB-NC 71.700 123.620 same as n2-c2-na

N\*-CK-NB 71.700 123.620 same as n2-c2-na

N\*-CK-H5 51.200 112.420 same as ha-c2-na

CB-N\*-CK 67.800 110.370 same as c2-na-c2

CB-CB-C 67.900 120.700 same as c -c2-c2

CB-CB-NB 70.000 113.420 same as cc-cc-nc

CB-NC-CA 69.426 110.070 Calculated with empirical approach

CB-NC-CA 68.600 110.190 same as cc-nc-cc

CB-CB-NC 70.000 113.420 same as cc-cc-nc

CB-C -O 72.800 119.120 same as c2-c -o

CB-C -NA 0.000 0.000 ATTN, need revision

CB-NB-CK 68.600 110.190 same as cc-nc-cc

C -CB-NB 69.987 116.350 Calculated with empirical approach

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-CA 64.300 125.090 same as c -na-c2

O -C -NA 75.000 122.850 same as na-c -o

NA-CA-N2 73.125 113.900 Calculated with empirical approach

NA-CA-NC 71.700 123.620 same as n2-c2-na

H -NA-CA 47.600 119.280 same as c2-na-hn

CA-N2-H 49.100 119.380 same as c2-n3-hn

N2-CA-NC 72.800 118.860 same as nc-ca-nh

H -N2-H 41.300 107.130 same as hn-n3-hn

NB-CK-H5 52.400 120.540 same as ha-c2-n2

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3

OS-CT-CT-HC 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-N\*-CB 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CB 1 2.500 0.000 1.000 same as os-c3-na-c2

OS-CT-N\*-CK 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CK 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-CB-CB 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CB-NC 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CK-NB 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CK-H5 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-CB 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CK 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CB 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CK 1 0.000 0.000 2.000 same as X -c3-na-X

HC-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

HC-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CB-CB-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CB-CB-NB 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CB-NC-CA 1 4.150 180.000 2.000 same as X -c2-n2-X

N\*-CK-NB-CB 1 4.150 180.000 2.000 same as X -c2-n2-X

CB-N\*-CK-NB 1 0.625 180.000 2.000 same as X -c2-na-X

CB-N\*-CK-H5 1 0.625 180.000 2.000 same as X -c2-na-X

CB-CB-C -O 1 2.175 180.000 -2.000 same as c2-c2-c -o

CB-CB-C -O 1 0.300 0.000 3.000 same as c2-c2-c -o

CB-CB-C -NA 1 2.175 180.000 2.000 same as X -c -c2-X

CB-CB-NB-CK 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-NC-CA-NA 1 4.150 180.000 2.000 same as X -c2-n2-X

CB-NC-CA-N2 1 4.800 180.000 2.000 same as X -ca-nc-X

CB-CB-N\*-CK 1 0.625 180.000 2.000 same as X -c2-na-X

CB-CB-NC-CA 1 4.750 180.000 2.000 same as X -cc-nc-X

CB-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

CB-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

CB-C -NA-CA 1 1.450 180.000 -2.000 same as X -c -na-X

CB-C -NA-CA 1 0.350 180.000 4.000 same as X -c -na-X

CB-NB-CK-H5 1 4.750 180.000 2.000 same as X -cc-nc-X

C -CB-CB-NC 1 6.650 180.000 2.000 same as X -c2-c2-X

C -CB-NB-CK 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NA-CA-N2 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-CA-NC 1 0.625 180.000 2.000 same as X -c2-na-X

O -C -CB-NB 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-CA 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-CA 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CB-NB 1 2.175 180.000 2.000 same as X -c -c2-X

NA-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

H -NA-CA-N2 1 0.625 180.000 2.000 same as X -c2-na-X

H -NA-CA-NC 1 0.625 180.000 2.000 same as X -c2-na-X

H -N2-CA-NC 1 0.300 180.000 2.000 same as X -c2-n3-X

NB-CB-CB-NC 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CB-N\*-CK 1 0.625 180.000 2.000 same as X -c2-na-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 HC 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 CB 1.9080 0.0860 same as cc

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CA 1.9080 0.0860 same as ca

 N2 1.8240 0.1700 same as nh

 NB 1.8240 0.1700 same as nc

 NC 1.8240 0.1700 same as nc

 CK 1.9080 0.0860 same as cc

 H5 1.4870 0.0157 same as hc

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frcmod.CDS:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

HC 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NC 14.010 0.530 same as n2

CA 12.010 0.360 same as c2

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

H4 1.008 0.135 same as ha

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

CT-HC 337.30 1.092 same as c3-hc

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NC 374.60 1.420 same as c -n2

NC-CA 492.90 1.336 same as ca-nc

CA-CM 411.70 1.434 same as ca-cc

CA-N2 449.00 1.364 same as ca-nh

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

N2-H 394.10 1.018 same as hn-n3

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-H1 46.400 110.050 same as c3-c3-hc

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-CT-HC 46.400 110.050 same as c3-c3-hc

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

HC-CT-HC 39.400 108.350 same as hc-c3-hc

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NC 70.700 118.600 same as n2-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NC-CA 66.200 120.970 same as c -n2-c2

O -C -NC 73.000 122.500 same as n2-c -o

NC-CA-CM 70.000 113.420 same as cc-cc-nc

NC-CA-N2 72.800 118.860 same as nc-ca-nh

CA-CM-HA 50.300 119.700 same as c2-c2-hc

CA-CM-CM 67.700 111.040 same as ca-cc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

CM-CA-N2 68.600 118.980 same as cc-cc-nh

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

H -N2-H 41.300 107.130 same as hn-n3-hn

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-H1 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

CT-CT-CT-HC 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-OS-CT 1 0.383 0.000 3.000 same as X -c3-os-X

OS-CT-CT-HC 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NC 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NC 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

HC-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

HC-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

N\*-CM-CM-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NC-CA-CM 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NC-CA-N2 1 4.150 180.000 2.000 same as X -c2-n2-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

NC-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NC-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NC-CA-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

NC-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CA-CM-CM-H4 1 4.000 180.000 2.000 same as X -cc-cc-X

CM-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

HA-CM-CA-N2 1 6.650 180.000 2.000 same as X -c2-c2-X

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

N2-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 HC 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NC 1.8240 0.1700 same as nc

 CA 1.9080 0.0860 same as ca

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 H4 1.4870 0.0157 same as hc

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frcmod.TLS:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CM 12.010 0.360 same as c2

HC 1.008 0.135 same as hc

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

C -CM 449.90 1.406 same as c -c2

CM-CT 328.30 1.508 same as c2-c3

CM-CM 418.30 1.429 same as cc-cc

CT-HC 337.30 1.092 same as c3-hc

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NA 73.200 115.400 same as na-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-C 64.700 126.400 same as c -na-c

O -C -NA 75.000 122.850 same as na-c -o

NA-C -CM 0.000 0.000 ATTN, need revision

C -CM-CT 63.900 119.700 same as c -c2-c3

C -CM-CM 67.900 120.700 same as c -c2-c2

O -C -CM 72.800 119.120 same as c2-c -o

CM-CT-HC 47.000 110.490 same as c2-c3-hc

CM-CM-H4 50.000 120.940 same as c2-c2-ha

CT-CM-CM 64.300 123.420 same as c2-c2-c3

HC-CT-HC 39.400 108.350 same as hc-c3-hc

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NA 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NA 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

N\*-C -NA-C 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-C 1 0.350 180.000 4.000 same as X -c -na-X

N\*-CM-CM-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-CT 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -O 1 0.350 180.000 4.000 same as X -c -na-X

C -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NA-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CM-CT 1 2.175 180.000 2.000 same as X -c -c2-X

NA-C -CM-CM 1 2.175 180.000 2.000 same as X -c -c2-X

H -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

H -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

C -CM-CT-HC 1 0.000 0.000 2.000 same as X -c2-c3-X

C -CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

O -C -CM-CT 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -CM-CM 1 2.175 180.000 -2.000 same as c2-c2-c -o

O -C -CM-CM 1 0.300 0.000 3.000 same as c2-c2-c -o

CT-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

HC-CT-CM-CM 1 0.380 180.000 -3.000 same as hc-c3-c2-c2

HC-CT-CM-CM 1 1.150 0.000 1.000 same as hc-c3-c2-c2

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CM 1.9080 0.0860 same as cc

 HC 1.4870 0.0157 same as hc

 H4 1.4870 0.0157 same as hc

----------------------------------------------------------------------------------------------------------

frcmod.mCLS:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NC 14.010 0.530 same as n2

CA 12.010 0.360 same as c2

CM 12.010 0.360 same as c2

HC 1.008 0.135 same as hc

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NC 374.60 1.420 same as c -n2

NC-CA 492.90 1.336 same as ca-nc

CA-CM 411.70 1.434 same as ca-cc

CA-N2 449.00 1.364 same as ca-nh

CM-CT 328.30 1.508 same as c2-c3

CM-CM 418.30 1.429 same as cc-cc

CT-HC 337.30 1.092 same as c3-hc

N2-H 394.10 1.018 same as hn-n3

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NC 70.700 118.600 same as n2-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NC-CA 66.200 120.970 same as c -n2-c2

O -C -NC 73.000 122.500 same as n2-c -o

NC-CA-CM 70.000 113.420 same as cc-cc-nc

NC-CA-N2 72.800 118.860 same as nc-ca-nh

CA-CM-CT 64.300 123.420 same as c2-c2-c3

CA-CM-CM 67.700 111.040 same as ca-cc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

CM-CA-N2 68.600 118.980 same as cc-cc-nh

CM-CT-HC 47.000 110.490 same as c2-c3-hc

CM-CM-H4 50.000 120.940 same as c2-c2-ha

CT-CM-CM 64.300 123.420 same as c2-c2-c3

HC-CT-HC 39.400 108.350 same as hc-c3-hc

H -N2-H 41.300 107.130 same as hn-n3-hn

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NC 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NC 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

N\*-CM-CM-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-CT 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NC-CA-CM 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NC-CA-N2 1 4.150 180.000 2.000 same as X -c2-n2-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

NC-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NC-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NC-CA-CM-CT 1 6.650 180.000 2.000 same as X -c2-c2-X

NC-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CA-CM-CT-HC 1 0.380 180.000 -3.000 same as hc-c3-c2-c2

CA-CM-CT-HC 1 1.150 0.000 1.000 same as hc-c3-c2-c2

CA-CM-CM-H4 1 4.000 180.000 2.000 same as X -cc-cc-X

CM-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CT-CM-CA-N2 1 6.650 180.000 2.000 same as X -c2-c2-X

CT-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

HC-CT-CM-CM 1 0.380 180.000 -3.000 same as hc-c3-c2-c2

HC-CT-CM-CM 1 1.150 0.000 1.000 same as hc-c3-c2-c2

N2-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NC 1.8240 0.1700 same as nc

 CA 1.9080 0.0860 same as ca

 CM 1.9080 0.0860 same as cc

 HC 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 H4 1.4870 0.0157 same as hc

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frcmod.RMC:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NC 14.010 0.530 same as n2

CA 12.010 0.360 same as c2

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NC 374.60 1.420 same as c -n2

NC-CA 492.90 1.336 same as ca-nc

CA-CM 411.70 1.434 same as ca-cc

CA-N2 449.00 1.364 same as ca-nh

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

N2-H 394.10 1.018 same as hn-n3

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NC 70.700 118.600 same as n2-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NC-CA 66.200 120.970 same as c -n2-c2

O -C -NC 73.000 122.500 same as n2-c -o

NC-CA-CM 70.000 113.420 same as cc-cc-nc

NC-CA-N2 72.800 118.860 same as nc-ca-nh

CA-CM-HA 50.300 119.700 same as c2-c2-hc

CA-CM-CM 67.700 111.040 same as ca-cc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

CM-CA-N2 68.600 118.980 same as cc-cc-nh

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

H -N2-H 41.300 107.130 same as hn-n3-hn

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NC 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NC 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

N\*-CM-CM-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NC-CA-CM 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NC-CA-N2 1 4.150 180.000 2.000 same as X -c2-n2-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

NC-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NC-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NC-CA-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

NC-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CA-CM-CM-H4 1 4.000 180.000 2.000 same as X -cc-cc-X

CM-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

HA-CM-CA-N2 1 6.650 180.000 2.000 same as X -c2-c2-X

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

N2-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NC 1.8240 0.1700 same as nc

 CA 1.9080 0.0860 same as ca

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 H4 1.4870 0.0157 same as hc

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frcmod.RMU:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

H4 1.008 0.135 same as ha

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

C -CM 449.90 1.406 same as c -c2

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NA 73.200 115.400 same as na-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-C 64.700 126.400 same as c -na-c

O -C -NA 75.000 122.850 same as na-c -o

NA-C -CM 0.000 0.000 ATTN, need revision

C -CM-HA 48.000 119.700 same as c -c2-hc

C -CM-CM 67.900 120.700 same as c -c2-c2

O -C -CM 72.800 119.120 same as c2-c -o

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NA 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NA 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

N\*-C -NA-C 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-C 1 0.350 180.000 4.000 same as X -c -na-X

N\*-CM-CM-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -O 1 0.350 180.000 4.000 same as X -c -na-X

C -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NA-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

NA-C -CM-CM 1 2.175 180.000 2.000 same as X -c -c2-X

H -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

H -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

C -CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

O -C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -CM-CM 1 2.175 180.000 -2.000 same as c2-c2-c -o

O -C -CM-CM 1 0.300 0.000 3.000 same as c2-c2-c -o

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 H4 1.4870 0.0157 same as hc

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frcmod.RMC:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NC 14.010 0.530 same as n2

CA 12.010 0.360 same as c2

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NC 374.60 1.420 same as c -n2

NC-CA 492.90 1.336 same as ca-nc

CA-CM 411.70 1.434 same as ca-cc

CA-N2 449.00 1.364 same as ca-nh

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

N2-H 394.10 1.018 same as hn-n3

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NC 70.700 118.600 same as n2-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NC-CA 66.200 120.970 same as c -n2-c2

O -C -NC 73.000 122.500 same as n2-c -o

NC-CA-CM 70.000 113.420 same as cc-cc-nc

NC-CA-N2 72.800 118.860 same as nc-ca-nh

CA-CM-HA 50.300 119.700 same as c2-c2-hc

CA-CM-CM 67.700 111.040 same as ca-cc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

CM-CA-N2 68.600 118.980 same as cc-cc-nh

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

H -N2-H 41.300 107.130 same as hn-n3-hn

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NC 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NC 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

N\*-CM-CM-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NC-CA-CM 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NC-CA-N2 1 4.150 180.000 2.000 same as X -c2-n2-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

NC-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NC-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NC-CA-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

NC-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CA-CM-CM-H4 1 4.000 180.000 2.000 same as X -cc-cc-X

CM-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

HA-CM-CA-N2 1 6.650 180.000 2.000 same as X -c2-c2-X

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

N2-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NC 1.8240 0.1700 same as nc

 CA 1.9080 0.0860 same as ca

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 H4 1.4870 0.0157 same as hc

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frcmod.RMU:

remark goes here

MASS

P 30.970 1.538 same as p4

SH 32.060 2.900 same as sh

O2 16.000 0.434 same as o

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

H4 1.008 0.135 same as ha

BOND

P -SH 163.10 2.115 same as p4-sh

P -O2 456.40 1.503 same as o -p4

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

C -CM 449.90 1.406 same as c -c2

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

SH-P -O2 37.000 118.090 same as o -p4-sh

SH-P -OS 52.589 99.575 Calculated with empirical approach

O2-P -OS 43.100 116.670 same as o -p4-os

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

H1-CT-CT 33.235 109.490 Calculated with empirical approach

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NA 73.200 115.400 same as na-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-C 64.700 126.400 same as c -na-c

O -C -NA 75.000 122.850 same as na-c -o

NA-C -CM 0.000 0.000 ATTN, need revision

C -CM-HA 48.000 119.700 same as c -c2-hc

C -CM-CM 67.900 120.700 same as c -c2-c2

O -C -CM 72.800 119.120 same as c2-c -o

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NA 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NA 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

N\*-C -NA-C 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-C 1 0.350 180.000 4.000 same as X -c -na-X

N\*-CM-CM-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -O 1 0.350 180.000 4.000 same as X -c -na-X

C -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NA-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

NA-C -CM-CM 1 2.175 180.000 2.000 same as X -c -c2-X

H -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

H -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

C -CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

O -C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -CM-CM 1 2.175 180.000 -2.000 same as c2-c2-c -o

O -C -CM-CM 1 0.300 0.000 3.000 same as c2-c2-c -o

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 SH 2.0000 0.2500 same as sh

 O2 1.6612 0.2100 same as o

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 H4 1.4870 0.0157 same as hc

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frcmod.CMS:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NC 14.010 0.530 same as n2

CA 12.010 0.360 same as c2

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

N2 14.010 0.530 same as n3

H 1.008 0.161 same as hn

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NC 374.60 1.420 same as c -n2

NC-CA 492.90 1.336 same as ca-nc

CA-CM 411.70 1.434 same as ca-cc

CA-N2 449.00 1.364 same as ca-nh

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

N2-H 394.10 1.018 same as hn-n3

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-H1 46.400 110.050 same as c3-c3-hc

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NC 70.700 118.600 same as n2-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NC-CA 66.200 120.970 same as c -n2-c2

O -C -NC 73.000 122.500 same as n2-c -o

NC-CA-CM 70.000 113.420 same as cc-cc-nc

NC-CA-N2 72.800 118.860 same as nc-ca-nh

CA-CM-HA 50.300 119.700 same as c2-c2-hc

CA-CM-CM 67.700 111.040 same as ca-cc-cc

CA-N2-H 49.100 119.380 same as c2-n3-hn

CM-CA-N2 68.600 118.980 same as cc-cc-nh

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

H -N2-H 41.300 107.130 same as hn-n3-hn

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-H1 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

H1-CT-OS-CT 1 0.383 0.000 3.000 same as X -c3-os-X

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NC 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NC 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

N\*-CM-CM-CA 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NC-CA-CM 1 4.150 180.000 2.000 same as X -c2-n2-X

C -NC-CA-N2 1 4.150 180.000 2.000 same as X -c2-n2-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NC-CA 1 4.150 180.000 2.000 same as X -c -n2-X

NC-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NC-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NC-CA-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

NC-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

NC-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

CA-CM-CM-H4 1 4.000 180.000 2.000 same as X -cc-cc-X

CM-CA-N2-H 1 0.300 180.000 2.000 same as X -c2-n3-X

HA-CM-CA-N2 1 6.650 180.000 2.000 same as X -c2-c2-X

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

N2-CA-CM-CM 1 4.000 180.000 2.000 same as X -cc-cc-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NC 1.8240 0.1700 same as nc

 CA 1.9080 0.0860 same as ca

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 N2 1.8240 0.1700 same as nh

 H 0.6000 0.0157 same as hn

 H4 1.4870 0.0157 same as hc

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frcmod.UMS:

remark goes here

MASS

P 30.970 1.538 same as p4

O2 16.000 0.434 same as o

SH 32.060 2.900 same as sh

OS 16.000 0.465 same as os

CT 12.010 0.878 same as c3

H1 1.008 0.135 same as hc

H2 1.008 0.135 same as hc

N\* 14.010 0.530 same as na

C 12.010 0.616 same as c

O 16.000 0.434 same as o

NA 14.010 0.530 same as na

H 1.008 0.161 same as hn

CM 12.010 0.360 same as c2

HA 1.008 0.135 same as hc

H4 1.008 0.135 same as ha

BOND

P -O2 456.40 1.503 same as o -p4

P -SH 163.10 2.115 same as p4-sh

P -OS 311.60 1.636 same as os-p4

OS-CT 301.50 1.439 same as c3-os

CT-H1 337.30 1.092 same as c3-hc

CT-CT 303.10 1.535 same as c3-c3

CT-H2 337.30 1.092 same as c3-hc

CT-N\* 334.70 1.456 same as c3-na

N\*-C 0.00 0.000 ATTN, need revision

N\*-CM 411.10 1.391 same as c2-na

C -O 648.00 1.214 same as c -o

C -NA 0.00 0.000 ATTN, need revision

NA-H 406.60 1.011 same as hn-na

C -CM 449.90 1.406 same as c -c2

CM-HA 344.30 1.087 same as c2-hc

CM-CM 418.30 1.429 same as cc-cc

CM-H4 344.30 1.087 same as c2-ha

ANGLE

P -OS-CT 77.600 117.480 same as c3-os-p4

O2-P -SH 37.000 118.090 same as o -p4-sh

O2-P -OS 43.100 116.670 same as o -p4-os

SH-P -OS 52.589 99.575 Calculated with empirical approach

OS-CT-H1 50.900 108.700 same as hc-c3-os

OS-CT-CT 67.800 108.420 same as c3-c3-os

CT-CT-H1 46.400 110.050 same as c3-c3-hc

CT-CT-CT 63.200 110.630 same as c3-c3-c3

H1-CT-H1 39.400 108.350 same as hc-c3-hc

CT-OS-CT 62.100 113.410 same as c3-os-c3

OS-CT-H2 50.900 108.700 same as hc-c3-os

OS-CT-N\* 71.200 109.190 same as na-c3-os

CT-N\*-C 64.700 117.600 same as c -na-c3

CT-N\*-CM 64.200 117.200 same as c2-na-c3

H2-CT-CT 46.400 110.050 same as c3-c3-hc

H2-CT-N\* 49.900 109.500 same as hc-c3-na

CT-CT-N\* 65.800 112.590 same as c3-c3-na

N\*-C -O 75.000 122.850 same as na-c -o

N\*-C -NA 73.200 115.400 same as na-c -na

N\*-CM-CM 69.800 121.380 same as c2-c2-na

N\*-CM-H4 51.200 112.420 same as ha-c2-na

C -N\*-CM 64.300 125.090 same as c -na-c2

C -NA-H 48.800 118.000 same as c -na-hn

C -NA-C 64.700 126.400 same as c -na-c

O -C -NA 75.000 122.850 same as na-c -o

NA-C -CM 0.000 0.000 ATTN, need revision

C -CM-HA 48.000 119.700 same as c -c2-hc

C -CM-CM 67.900 120.700 same as c -c2-c2

O -C -CM 72.800 119.120 same as c2-c -o

CM-CM-H4 50.000 120.940 same as c2-c2-ha

HA-CM-CM 50.300 119.700 same as c2-c2-hc

DIHE

P -OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X

P -OS-CT-CT 1 0.383 0.000 3.000 same as X -c3-os-X

O2-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

SH-P -OS-CT 1 1.050 180.000 2.000 same as X -os-p4-X

OS-CT-CT-H1 1 0.250 0.000 1.000 same as hc-c3-c3-os

OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os

OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os

OS-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

CT-CT-OS-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3

CT-CT-OS-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3

CT-CT-CT-CT 1 0.180 0.000 -3.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3

CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3

CT-CT-CT-H1 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

CT-OS-CT-H2 1 0.383 0.000 3.000 same as X -c3-os-X

CT-OS-CT-N\* 1 0.383 0.000 -3.000 same as c3-os-c3-na

CT-OS-CT-N\* 1 0.650 0.000 2.000 same as c3-os-c3-na

H1-CT-OS-CT 1 0.383 0.000 3.000 same as X -c3-os-X

OS-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

OS-CT-N\*-CM 1 0.000 0.000 -2.000 same as os-c3-na-c2

OS-CT-N\*-CM 1 2.500 0.000 1.000 same as os-c3-na-c2

CT-N\*-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -O 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-C -NA 1 1.450 180.000 -2.000 same as X -c -na-X

CT-N\*-C -NA 1 0.350 180.000 4.000 same as X -c -na-X

CT-N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

CT-N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

H2-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc

H2-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os

H2-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3

H2-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

H2-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-C 1 0.000 0.000 2.000 same as X -c3-na-X

CT-CT-N\*-CM 1 0.000 0.000 2.000 same as X -c3-na-X

H1-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

OS-CT-CT-N\* 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-CT-CT-CT 1 0.156 0.000 3.000 same as X -c3-c3-X

N\*-C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

N\*-C -NA-C 1 1.450 180.000 -2.000 same as X -c -na-X

N\*-C -NA-C 1 0.350 180.000 4.000 same as X -c -na-X

N\*-CM-CM-C 1 6.650 180.000 2.000 same as X -c2-c2-X

N\*-CM-CM-HA 1 6.650 180.000 2.000 same as X -c2-c2-X

C -N\*-CM-CM 1 0.625 180.000 2.000 same as X -c2-na-X

C -N\*-CM-H4 1 0.625 180.000 2.000 same as X -c2-na-X

C -NA-C -O 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -O 1 0.350 180.000 4.000 same as X -c -na-X

C -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

C -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X

O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -N\*-CM 1 1.450 180.000 -2.000 same as X -c -na-X

NA-C -N\*-CM 1 0.350 180.000 4.000 same as X -c -na-X

NA-C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

NA-C -CM-CM 1 2.175 180.000 2.000 same as X -c -c2-X

H -NA-C -CM 1 1.450 180.000 -2.000 same as X -c -na-X

H -NA-C -CM 1 0.350 180.000 4.000 same as X -c -na-X

C -CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

O -C -CM-HA 1 2.175 180.000 2.000 same as X -c -c2-X

O -C -CM-CM 1 2.175 180.000 -2.000 same as c2-c2-c -o

O -C -CM-CM 1 0.300 0.000 3.000 same as c2-c2-c -o

HA-CM-CM-H4 1 6.650 180.000 2.000 same as X -c2-c2-X

IMPROPER

NONBON

 P 2.1000 0.2000 same as p4

 O2 1.6612 0.2100 same as o

 SH 2.0000 0.2500 same as sh

 OS 1.6837 0.1700 same as os

 CT 1.9080 0.1094 same as c3

 H1 1.4870 0.0157 same as hc

 H2 1.4870 0.0157 same as hc

 N\* 1.8240 0.1700 same as na

 C 1.9080 0.0860 same as c

 O 1.6612 0.2100 same as o

 NA 1.8240 0.1700 same as na

 H 0.6000 0.0157 same as hn

 CM 1.9080 0.0860 same as cc

 HA 1.4870 0.0157 same as hc

 H4 1.4870 0.0157 same as hc

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PREPI Files

ADS.prepi:

0 0 0

leap-generated prep residue

ADS.res

ADS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 3.866999 3.597997 -1.386183 0.819388

 5 SP SH E 2.442535 4.024226 -1.406178 -0.174161

 6 O1P O2 E 4.266397 2.837809 -2.605066 -0.709250

 7 O5' OS M 4.838608 4.831727 -1.137217 -0.357456

 8 C5' CT M 4.904372 5.492922 0.127906 0.019164

 9 H5'1 H1 E 5.297536 4.808868 0.898686 0.059297

 10 H5'2 H1 E 3.888158 5.801902 0.417805 0.059297

 11 C4' CT M 5.819996 6.729552 -0.022080 0.050308

 12 H4' H1 E 5.568643 7.456047 0.768892 0.116518

 13 O4' OS S 7.161825 6.265079 0.170921 -0.384624

 14 C1' CT 3 7.807936 6.130309 -1.098780 0.224946

 15 H1' H2 E 8.596841 6.892093 -1.044766 0.064667

 16 C2' CT B 6.830683 6.529333 -2.230622 -0.097250

 17 H2'1 HC E 6.395438 5.645712 -2.713514 0.045165

 18 H2'2 HC E 7.355802 7.067443 -3.030805 0.045165

 19 N9 N\* B 8.539332 4.883567 -1.246777 -0.161278

 20 C4 CB B 9.869322 4.765212 -1.031751 0.541423

 21 C5 CB B 10.210874 3.461809 -1.331737 0.004928

 22 C6 CA B 11.532293 3.018418 -1.223753 0.850376

 23 N1 NC S 12.428685 3.945212 -0.813700 -0.840581

 24 C2 CQ S 12.075363 5.221403 -0.521748 0.576905

 25 H2 H5 E 12.832866 5.926642 -0.202818 0.083715

 26 N6 N2 B 11.900799 1.752651 -1.509828 -1.029216

 27 H61 H E 12.888860 1.474632 -1.412856 0.443535

 28 H62 H E 11.204996 1.059236 -1.822868 0.443535

 29 N7 NB E 9.065125 2.872751 -1.696690 -0.675565

 30 N3 NC E 10.796742 5.646979 -0.617741 -0.804899

 31 C8 CK S 8.111583 3.712950 -1.643705 0.263528

 32 H8 H5 E 7.082641 3.468933 -1.903810 0.168820

 33 C3' CT M 5.740862 7.327536 -1.456405 0.333274

 34 H3' H1 E 4.737154 7.153646 -1.879419 0.027275

 35 O3' OS M 5.807176 8.770860 -1.477423 -0.504450

LOOP

 C2' C3'

 C2 N3

 C8 N7

IMPROPER

DONE

STOP

----------------------------------------------------------------------------------------------------------

TDS.prepi:

0 0 0

leap-generated prep residue

TDS.res

TDS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 2.029782 2.776684 -1.584584 0.837378

 5 SP SH E 0.607650 3.169129 -1.735640 -0.184314

 6 O1P O2 E 2.474286 1.947669 -2.741403 -0.699180

 7 O5' OS M 2.995465 4.042576 -1.426550 -0.221420

 8 C5' CT M 3.105014 4.814733 -0.219594 -0.193890

 9 H5'1 H1 E 3.446034 4.197633 0.626038 0.124566

 10 H5'2 H1 E 2.099183 5.187880 0.023441 0.124566

 11 C4' CT M 4.103595 5.990338 -0.408546 0.181150

 12 H4' H1 E 3.865196 6.766716 0.336308 0.095727

 13 O4' OS S 5.425498 5.477816 -0.156565 -0.419183

 14 C1' CT 3 6.195405 5.439267 -1.369300 0.217903

 15 H1' H2 E 6.875515 6.294140 -1.310322 0.084207

 16 C2' CT B 5.217328 5.734309 -2.543877 -0.118361

 17 H2'1 HC E 4.753777 4.843060 -2.982070 0.058921

 18 H2'2 HC E 5.730620 6.223485 -3.382234 0.058921

 19 N1 N\* B 7.017566 4.225936 -1.432295 -0.272299

 20 C2 C B 8.336311 4.251267 -1.074334 0.831265

 21 O2 O E 8.878297 5.276055 -0.675416 -0.628021

 22 N3 NA B 9.087485 3.127518 -1.153344 -0.754618

 23 H3 H E 10.059136 3.147318 -0.909406 0.436253

 24 C4 C B 8.563631 1.956468 -1.557380 0.748566

 25 O4 O E 9.187822 0.912199 -1.648416 -0.595102

 26 C5 CM S 7.149665 1.964837 -1.900388 0.079490

 27 C7 CT 3 6.469151 0.700818 -2.335309 -0.655058

 28 H71 HC E 6.287724 1.496253 -3.076099 0.178344

 29 H72 HC E 7.548599 0.501804 -2.263300 0.178344

 30 H73 HC E 6.117471 1.031225 -1.350138 0.178344

 31 C6 CM S 6.427559 3.075565 -1.824391 -0.119304

 32 H6 H4 E 5.384245 2.951680 -2.095266 0.223998

 33 C3' CT M 4.080563 6.540370 -1.860697 0.190066

 34 H3' H1 E 3.096304 6.332610 -2.315545 0.102011

 35 O3' OS M 4.116887 7.983856 -1.954710 -0.484971

LOOP

 C2' C3'

 C5 C6

IMPROPER

DONE

STOP

----------------------------------------------------------------------------------------------------------

GDS.prepi:

0 0 0

leap-generated prep residue

GDS.res

GDS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 1.805968 2.825657 -1.293925 0.807444

 5 SP SH E 0.384381 3.241948 -1.247934 -0.188520

 6 O1P O2 E 2.115396 2.114035 -2.568253 -0.689781

 7 O5' OS M 2.781618 4.075473 -1.102944 -0.165002

 8 C5' CT M 3.002237 4.794771 0.117832 -0.238832

 9 H5'1 H1 E 3.408369 4.152665 0.914675 0.134871

 10 H5'2 H1 E 2.025618 5.165921 0.458806 0.134871

 11 C4' CT M 3.987723 5.968243 -0.128100 0.120170

 12 O4' OS S 5.325295 5.456902 0.013859 -0.424906

 13 C1' CT 3 5.946457 5.326086 -1.271987 0.270171

 14 H1' H2 E 6.746727 6.079282 -1.263985 0.060214

 15 C2' CT B 4.891017 5.678122 -2.355970 -0.276102

 16 H2'1 HC E 4.331673 4.807103 -2.709943 0.088832

 17 H2'2 HC E 5.346900 6.217839 -3.197799 0.088832

 18 N9 N\* B 6.612831 4.046385 -1.459974 0.009781

 19 C4 CB B 7.894390 3.819992 -1.277161 0.215679

 20 C5 CB B 8.204829 2.552988 -1.549024 0.157503

 21 C6 C B 9.575718 2.074562 -1.406010 0.630805

 22 O6 O E 9.835826 0.904411 -1.632922 -0.580588

 23 N1 NA B 10.483056 3.009348 -1.018976 -0.707252

 24 H1 H E 11.429695 2.696093 -0.930963 0.389953

 25 C2 CA S 10.152674 4.315555 -0.760029 1.003108

 26 N2 N2 B 11.106377 5.137516 -0.412946 -1.088741

 27 H21 H E 12.085212 4.820246 -0.333914 0.459749

 28 H22 H E 10.890550 6.128073 -0.219971 0.459749

 29 N7 NB E 6.931644 2.027523 -1.948079 -0.650046

 30 N3 NC E 8.940070 4.716246 -0.860024 -0.771766

 31 C8 CK S 6.067773 2.941078 -1.883077 0.195268

 32 H8 H5 E 5.031972 2.767107 -2.163114 0.158839

 33 C3' CT M 3.859642 6.541007 -1.569167 0.291303

 34 H3' H1 E 2.825310 6.399122 -1.925026 0.079789

 35 O3' OS M 3.966928 7.977995 -1.623179 -0.512691

LOOP

 C2' C3'

 C2 N3

 C8 N7

IMPROPER

DONE

STOP

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CDS.prepi:

0 0 0

leap-generated prep residue

CDS.res

CDS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 1.891283 2.808013 -1.433372 0.774765

 5 SP SH E 0.459084 3.193446 -1.483390 -0.170895

 6 O1P O2 E 2.283606 2.071876 -2.669198 -0.689912

 7 O5' OS M 2.836080 4.082073 -1.223303 -0.165563

 8 C5' CT M 2.963727 4.813499 0.007019 -0.277061

 9 H5'1 H1 E 3.329005 4.181030 0.832221 0.144304

 10 H5'2 H1 E 1.959778 5.166705 0.285104 0.144304

 11 C4' CT M 3.941457 6.008336 -0.169967 0.231560

 12 H4' H1 E 3.717981 6.751098 0.614235 0.086873

 13 O4' OS S 5.279526 5.522824 0.027056 -0.404200

 14 C1' CT 3 5.979627 5.455165 -1.224893 0.047030

 15 H1' H2 E 6.721300 6.262799 -1.167868 0.109337

 16 C2' CT B 4.984535 5.835492 -2.357665 -0.024309

 17 H2'1 HC E 4.503980 4.985269 -2.852856 0.037235

 18 H2'2 HC E 5.503594 6.361541 -3.169733 0.037235

 19 N1 N\* B 6.711242 4.194182 -1.334923 -0.230733

 20 C2 C B 8.015245 4.111627 -0.978210 0.934759

 21 O2 O E 8.669434 5.061854 -0.566228 -0.638422

 22 N3 NC S 8.721424 2.863282 -1.067176 -0.925786

 23 C4 CA B 8.151452 1.797226 -1.466157 1.183057

 24 C5 CM S 6.723592 1.898487 -1.826072 -0.808969

 25 H5 HA E 6.176251 1.015422 -2.159080 0.229170

 26 N4 N2 B 8.780703 0.662246 -1.558160 -1.160964

 27 H41 H E 9.778537 0.605162 -1.309225 0.472546

 28 H42 H E 8.290359 -0.185616 -1.880115 0.472546

 29 C6 CM S 6.079181 3.068615 -1.750054 0.238368

 30 H6 H4 E 5.032532 3.044617 -2.034965 0.153870

 31 C3' CT M 3.876331 6.613180 -1.598858 0.166855

 32 H3' H1 E 2.876467 6.425258 -2.024965 0.096029

 33 O3' OS M 3.930591 8.056890 -1.626845 -0.481628

LOOP

 C2' C3'

 C5 C6

IMPROPER

DONE

STOP

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mCLS.prepi:

0 0 0

leap-generated prep residue

mCLS.res

mCLS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P1 P M 3.204563 3.276929 -1.887770 1.159489

 5 O1P O2 E 3.496189 2.363770 -3.032385 -0.753107

 6 SP SH E 2.268598 4.395004 -2.239733 -0.413067

 7 O5' OS M 4.604991 3.930406 -1.461884 -0.436509

 8 C5' CT M 5.571647 4.501053 -2.352628 0.006216

 9 H5'1 H1 E 5.119901 5.331562 -2.916881 0.104929

 10 H5'2 H1 E 5.921988 3.733919 -3.060418 0.104929

 11 C4' CT M 6.765959 5.014430 -1.521417 0.060184

 12 O4' OS S 7.480037 3.966608 -0.845301 -0.386054

 13 C1' CT 3 8.716902 4.544910 -0.397305 0.320236

 14 H1' H2 E 8.766806 4.587003 0.700756 0.138648

 15 C2' CT B 8.650693 5.959636 -1.016808 0.096540

 16 H2'1 H1 E 9.634553 6.441387 -1.104769 0.160269

 17 O2' OS S 7.691946 6.713072 -0.254586 -0.465120

 18 C6' CT B 6.412974 6.091573 -0.468625 0.175689

 19 H6'1 H1 E 6.011841 5.642858 0.453301 0.049585

 20 H6'2 H1 E 5.706377 6.841429 -0.856747 0.049585

 21 N1 N\* B 9.750669 4.182813 -1.410358 -0.528211

 22 C2 C B 11.000587 4.314551 -0.785254 0.941640

 23 O2 O E 11.157954 5.140573 0.112423 -0.658878

 24 N3 NC S 12.040314 3.522326 -1.185300 -0.820849

 25 C4 CA B 11.819346 2.451912 -1.974282 0.796134

 26 C5 CM S 10.432159 2.143346 -2.405238 0.177642

 27 C7 CT 3 10.211815 1.232681 -2.952379 -0.558266

 28 H71 HC E 9.135500 1.190642 -3.175489 0.125273

 29 H72 HC E 10.493334 0.361531 -2.342588 0.125273

 30 H73 HC E 10.782901 1.221745 -3.892454 0.125273

 31 N4 N2 B 12.854550 1.681042 -2.363146 -1.000974

 32 H41 H E 13.789895 1.896757 -2.052213 0.452994

 33 H42 H E 12.705080 0.887906 -2.967014 0.452994

 34 C6 CM S 9.440840 3.026177 -2.100373 -0.104664

 35 H6 H4 E 8.414560 2.832305 -2.394289 0.228811

 36 C3' CT M 7.878319 5.706190 -2.323608 0.088516

 37 H3' H1 E 8.373668 5.015089 -3.024617 0.104430

 38 O3' OS M 7.381206 6.892931 -2.972458 -0.332558

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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TLS.prepi:

0 0 0

leap-generated prep residue

TLS.res

TLS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 8.159446 3.686840 -0.403819 0.862156

 5 O1P O2 E 7.742795 2.508344 0.408972 -0.692556

 6 SP SH E 9.361582 4.334307 0.172358 -0.182100

 7 O5' OS M 6.946793 4.723266 -0.513790 -0.318945

 8 C5' CT M 6.957542 5.901906 -1.330520 -0.471413

 9 H5'1 H1 E 7.744136 6.586323 -0.989562 0.209645

 10 H5'2 H1 E 7.166031 5.662264 -2.384704 0.209645

 11 C4' CT M 5.552556 6.532134 -1.217534 0.436685

 12 O4' OS S 4.583761 5.817469 -2.010020 -0.497478

 13 C1' CT 3 3.279991 6.126037 -1.484957 0.401820

 14 H1' H2 E 2.651963 6.569972 -2.274201 0.098146

 15 C2' CT B 3.648878 7.181428 -0.414267 -0.093191

 16 H2'1 H1 E 2.843184 7.401969 0.302963 0.177886

 17 O2' OS S 4.165811 8.360810 -1.065487 -0.401131

 18 C6' CT B 5.446706 8.017194 -1.626591 0.102426

 19 H6'1 H1 E 6.238710 8.617831 -1.148496 0.066115

 20 H6'2 H1 E 5.479429 8.163234 -2.716362 0.066115

 21 N1 N\* B 2.629313 4.935922 -0.861022 -0.186330

 22 C2 C B 1.300116 4.939389 -0.669004 0.740692

 23 O2 O E 0.711150 6.008164 -0.628008 -0.641360

 24 N3 NA B 0.594384 3.802220 -0.546020 -0.644704

 25 H3 H E -0.298920 3.952532 0.052988 0.393144

 26 C4 C B 1.278503 2.732361 -0.130956 0.767922

 27 O4 O E 0.691119 1.766905 0.339204 -0.621402

 28 C5 CM S 2.740695 2.680117 -0.272957 -0.104943

 29 C7 CT 3 3.536914 1.422858 -0.000002 -0.365470

 30 H71 HC E 2.914819 0.522980 -0.114969 0.124468

 31 H72 HC E 3.923968 1.452600 1.030292 0.124468

 32 H73 HC E 4.389276 1.333449 -0.691150 0.124468

 33 C6 CM S 3.328716 3.811531 -0.675079 -0.172969

 34 H6 H4 E 4.405845 3.763571 -0.828090 0.273898

 35 C3' CT M 4.919125 6.569797 0.187786 0.073741

 36 H3' H1 E 4.717047 5.592766 0.648629 0.089212

 37 O3' OS M 5.497448 7.491025 1.129912 -0.331093

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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RMC.prepi:

0 0 0

leap-generated prep residue

RMC.res

RMC INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 3.999717 3.009750 2.085163 1.220609

 5 O1P O2 E 3.683627 1.981062 3.114244 -0.774360

 6 S SH E 5.167538 3.830179 2.578307 -0.218466

 7 O5' OS M 2.648947 3.813373 1.765123 -0.507614

 8 C5' CT M 1.666933 4.252619 2.713315 -0.116823

 9 H5'1 H1 E 2.137847 4.928753 3.443578 0.121186

 10 H5'2 H1 E 1.250398 3.391545 3.256500 0.121186

 11 C4' CT M 0.532843 4.977326 1.948501 0.319322

 12 O4' OS S -0.223348 4.138192 1.079792 -0.362204

 13 C1' CT 3 -1.398915 4.895105 0.756759 0.030895

 14 H1' H2 E -1.485232 5.044007 -0.332731 0.168776

 15 C2' CT B -1.204900 6.216060 1.532698 0.085653

 16 H2'1 H1 E -2.104699 6.836138 1.658655 0.146275

 17 O2' OS S -0.164012 6.890096 0.824593 -0.392429

 18 C6' CT B 0.985818 6.039071 0.924606 -0.023645

 19 H6'1 H1 E 1.265531 5.615706 -0.058125 0.145881

 20 C7 CT 3 2.123480 6.870367 1.486710 0.337286

 21 H71 H1 E 3.027410 6.259201 1.589683 -0.063623

 22 H72 H1 E 1.844756 7.283760 2.460494 -0.063623

 23 O7 OS S 2.312531 7.920832 0.548614 -0.385176

 24 C8 CT 3 3.263947 8.845742 1.062694 0.001947

 25 H81 H1 E 3.428624 9.588349 0.276403 0.061750

 26 H82 H1 E 4.205574 8.326694 1.299608 0.061750

 27 H83 H1 E 2.863881 9.336170 1.966041 0.061750

 28 N1 N\* B -2.553309 4.216142 1.288610 -0.077944

 29 C2 C B -3.774854 4.679986 0.978241 0.810038

 30 O2 O E -3.949729 5.704274 0.329491 -0.634793

 31 N3 NC S -4.936104 3.954041 1.400133 -0.854805

 32 C4 CA B -4.833093 2.874549 2.066927 1.080759

 33 C5 CM S -3.479695 2.436227 2.467766 -0.670927

 34 H5 HA E -3.334060 1.546791 3.082563 0.209590

 35 N4 N2 B -5.869020 2.161425 2.388038 -1.113645

 36 H41 H E -6.809614 2.468666 2.102053 0.463366

 37 H42 H E -5.758408 1.282046 2.912784 0.463366

 38 C6 CM S -2.403203 3.119103 2.074826 0.035708

 39 H6 H4 E -1.439130 2.737767 2.420943 0.201542

 40 C3' CT M -0.522989 5.705372 2.815583 0.039677

 41 H3' H1 E -1.138883 5.017006 3.414773 0.079664

 42 O3' OS M 0.041244 6.707588 3.683734 -0.305955

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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RMU.prepi:

0 0 0

 leap-generated prep residue

RMU.res

RMU INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 4.597653 2.196788 2.256675 0.878677

 5 SP SH E 5.922193 2.515316 2.852749 -0.180252

 6 O1P O2 E 3.889427 1.163200 3.064879 -0.702957

 7 O5' OS M 3.666362 3.492836 2.198679 -0.297581

 8 C5' CT M 3.994198 4.640462 1.414675 -0.278449

 9 H5'1 H1 E 4.953682 5.006345 1.797736 0.172850

 10 H5'2 H1 E 4.136655 4.400719 0.349579 0.172850

 11 C4' CT M 2.813595 5.630022 1.556654 0.141161

 12 O4' OS S 1.706623 5.237047 0.735879 -0.379252

 13 C1' CT 3 0.562359 5.948146 1.226257 0.141368

 14 H1' H2 E 0.116322 6.577080 0.437523 0.154971

 15 C2' CT B 1.178796 6.800379 2.359315 0.018880

 16 H2'1 H1 E 0.462106 7.247956 3.065169 0.168116

 17 O2' OS S 2.008722 7.782664 1.722476 -0.370939

 18 C6' CT B 3.053943 7.062713 1.048568 0.098009

 19 H6'1 H1 E 2.976700 7.176616 -0.047828 0.122185

 20 C7 CT 3 4.415597 7.550126 1.535398 0.181564

 21 H71 H1 E 5.220626 7.123529 0.917220 0.006001

 22 H72 H1 E 4.567112 7.248522 2.576030 0.006001

 23 O7 OS S 4.397940 8.969820 1.456400 -0.353759

 24 C8 CT 3 5.534164 9.508059 2.133509 -0.043168

 25 H81 H1 E 5.519143 10.586538 1.956572 0.074354

 26 H82 H1 E 6.462037 9.070767 1.733472 0.074354

 27 H83 H1 E 5.463552 9.310941 3.216453 0.074354

 28 N1 N\* B -0.402085 4.980070 1.789429 -0.016036

 29 C2 C B -1.661610 5.381635 2.008381 0.686535

 30 O2 O E -1.892852 6.572227 2.140359 -0.616801

 31 N3 NA B -2.673019 4.502702 2.061395 -0.657302

 32 H3 H E -3.465787 4.886255 2.693425 0.385229

 33 C4 C B -2.328764 3.273530 2.452355 0.922178

 34 O4 O E -3.159551 2.508769 2.919494 -0.649309

 35 C5 CM S -0.951254 2.798249 2.311394 -0.620721

 36 H5 HA E -0.677355 1.757006 2.481372 0.247691

 37 C6 CM S -0.041999 3.703901 1.958394 -0.001952

 38 H6 H4 E 0.973937 3.325721 1.835364 0.228603

 39 C3' CT M 2.203199 5.829885 2.971712 -0.010129

 40 H3' H1 E 1.729946 4.934113 3.397652 0.113604

 41 O3' OS M 2.931879 6.504205 4.021637 -0.263419

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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SMC.prepi:

0 0 0

 leap-generated prep residue

SMC.res

SMC INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 3.784183 2.235193 2.529846 1.124800

 5 O1P O2 E 3.615745 0.890054 3.145760 -0.755275

 6 SP SH E 4.831588 2.996048 3.318705 -0.170617

 7 O5' OS M 2.345651 2.942593 2.474834 -0.418019

 8 C5' CT M 1.318704 3.078628 3.463519 -0.075885

 9 H5'1 H1 E 1.742783 3.557397 4.358470 0.105801

 10 H5'2 H1 E 0.946446 2.077582 3.722619 0.105801

 11 C4' CT M 0.160816 3.944654 2.902365 0.315356

 12 O4' OS S -0.523916 3.350486 1.792593 -0.394858

 13 C1' CT 3 -1.739475 4.101310 1.597548 0.041884

 14 H1' H2 E -1.803362 4.590045 0.610803 0.169899

 15 C2' CT B -1.665052 5.136571 2.741187 0.037574

 16 H2'1 H1 E -2.624954 5.625768 2.963162 0.160545

 17 O2' OS S -0.629010 6.077334 2.428237 -0.351274

 18 C6' CT B 0.600295 5.333697 2.400268 -0.030869

 19 H6'1 H1 E 1.332277 5.814017 3.071167 0.138727

 20 C7 CT 3 1.137460 5.234687 0.960390 0.150425

 21 H71 H1 E 0.421345 4.784348 0.260406 0.038278

 22 H72 H1 E 2.056369 4.638548 0.922429 0.038278

 23 O7 OS S 1.384882 6.569725 0.534497 -0.380060

 24 C8 CT 3 1.812967 6.586506 -0.829820 0.020126

 25 H81 H1 E 2.035081 7.631284 -1.070922 0.055590

 26 H82 H1 E 1.016557 6.215944 -1.496922 0.055590

 27 H83 H1 E 2.718087 5.972228 -0.954799 0.055590

 28 N1 N\* B -2.876119 3.211967 1.747587 -0.094976

 29 C2 C B -4.116583 3.667903 1.479569 0.825363

 30 O2 O E -4.340745 4.824492 1.147560 -0.630941

 31 N3 NC S -5.242171 2.777617 1.570597 -0.866922

 32 C4 CA B -5.099914 1.556934 1.902599 1.105872

 33 C5 CM S -3.736398 1.095587 2.233525 -0.689304

 34 H5 HA E -3.560421 0.068506 2.556663 0.209429

 35 N4 N2 B -6.097448 0.723022 1.948599 -1.130012

 36 H41 H E -7.047452 1.043403 1.712484 0.467598

 37 H42 H E -5.944675 -0.261338 2.210506 0.467598

 38 C6 CM S -2.693782 1.925653 2.139504 0.048455

 39 H6 H4 E -1.721556 1.498267 2.393631 0.213204

 40 C3' CT M -0.988462 4.313789 3.853328 0.041037

 41 H3' H1 E -1.573812 3.440743 4.184326 0.092318

 42 O3' OS M -0.494930 5.105796 4.947400 -0.318875

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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SMU.prepi:

0 0 0

 leap-generated prep residue

SMU.res

SMU INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M 4.323548 1.711397 2.508569 0.860659

 5 SP SH E 5.446413 2.311491 3.284548 -0.194288

 6 O1P O2 E 4.126243 0.279066 2.868564 -0.697222

 7 O5' OS M 2.979191 2.493797 2.861524 -0.302231

 8 C5' CT M 2.795635 3.870182 2.532584 -0.310678

 9 H5'1 H1 E 3.519460 4.515596 3.049612 0.164987

 10 H5'2 H1 E 2.936328 4.025436 1.451704 0.164987

 11 C4' CT M 1.338820 4.206491 2.901619 0.296275

 12 O4' OS S 0.461549 3.688700 1.892340 -0.401269

 13 C1' CT 3 -0.873423 3.763385 2.408696 0.140210

 14 H1' H2 E -1.519541 4.414104 1.795747 0.174316

 15 C2' CT B -0.621556 4.357841 3.815639 0.041334

 16 H2'1 H1 E -1.457097 4.250333 4.521411 0.163693

 17 O2' OS S -0.221124 5.728499 3.654641 -0.389328

 18 C6' CT B 1.053022 5.709864 2.992599 0.024235

 19 H6'1 H1 E 1.795716 6.241051 3.611352 0.138206

 20 C7 CT 3 0.968919 6.303680 1.579611 0.091732

 21 H71 H1 E 1.954899 6.272523 1.090658 0.050200

 22 H72 H1 E 0.247605 5.769084 0.942340 0.050200

 23 O7 OS S 0.494494 7.631640 1.791555 -0.342184

 24 C8 CT 3 0.209241 8.279178 0.552340 -0.005967

 25 H81 H1 E -0.120719 9.293740 0.803349 0.063711

 26 H82 H1 E -0.598008 7.757520 0.011200 0.063711

 27 H83 H1 E 1.117412 8.318870 -0.068829 0.063711

 28 N1 N\* B -1.421977 2.394137 2.484714 -0.076837

 29 C2 C B -2.738808 2.234673 2.681715 0.709542

 30 O2 O E -3.382592 3.148595 3.172765 -0.623681

 31 N3 NA B -3.364811 1.101293 2.332645 -0.666170

 32 H3 H E -4.234782 0.947630 2.960813 0.387942

 33 C4 C B -2.593574 0.010447 2.344658 0.932096

 34 O4 O E -3.082462 -1.103368 2.461649 -0.651430

 35 C5 CM S -1.140759 0.118170 2.199674 -0.623973

 36 H5 HA E -0.508012 -0.756800 2.043661 0.247582

 37 C6 CM S -0.624123 1.342979 2.266677 0.017882

 38 H6 H4 E 0.459255 1.401045 2.142640 0.223457

 39 C3' CT M 0.708956 3.698470 4.214231 0.052241

 40 H3' H1 E 0.615032 2.604552 4.296223 0.092396

 41 O3' OS M 1.182733 4.299243 5.432972 -0.337530

LOOP

 C2' C3'

 C4' C6'

 C5 C6

IMPROPER

DONE

STOP

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CMS.prepi:

0 0 0

 leap-generated prep residue

CMS.res

CMS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M -1.316809 -3.932303 0.271975 0.809417

 5 O1P O2 E -1.091178 -3.222960 1.563875 -0.695409

 6 SP SH E -2.334616 -4.998022 0.428930 -0.160234

 7 O5' OS M 0.050663 -4.531859 -0.300173 -0.180758

 8 C5' CT M 0.253566 -4.979560 -1.650493 -0.375343

 9 H5'1 H1 E 0.096085 -4.168098 -2.376255 0.144031

 10 H5'2 H1 E -0.490802 -5.761817 -1.849471 0.144031

 11 C4' CT M 1.685997 -5.540996 -1.854538 0.556486

 12 H4' H1 E 1.692298 -6.227181 -2.716811 0.036738

 13 O4' OS S 2.536113 -4.419088 -2.148593 -0.579169

 14 C1' CT 3 3.281255 -4.056783 -0.981863 0.160130

 15 H1' H2 E 4.292429 -4.365746 -1.262763 0.118042

 16 C2' CT B 2.826136 -5.002690 0.170681 0.313995

 17 H2'1 H1 E 2.089254 -4.604008 0.878825 -0.023498

 18 O2' OS S 3.929850 -5.358654 0.979693 -0.345410

 19 C10 CT 3 4.524960 -4.252227 1.666925 0.077270

 20 H101 H1 E 4.095951 -4.188078 2.676696 0.051917

 21 H102 H1 E 4.473078 -3.257079 1.205848 0.051917

 22 C11 CT 3 6.001137 -4.658566 1.613883 0.000784

 23 H111 H1 E 6.604591 -3.907624 2.142777 0.054832

 24 H112 H1 E 6.107032 -5.642822 2.098062 0.054832

 25 O11 OS S 6.360243 -4.746832 0.219070 -0.231830

 26 C12 CT 3 7.740123 -5.087285 0.036011 -0.138663

 27 H121 H1 E 7.957283 -5.170841 -1.039098 0.089021

 28 H122 H1 E 7.966915 -6.048749 0.519903 0.089021

 29 H123 H1 E 8.367597 -4.292148 0.465004 0.089021

 30 N1 N\* B 3.343511 -2.613984 -0.723904 -0.048490

 31 C2 C B 4.389828 -1.861878 -1.151733 0.865930

 32 O2 O E 5.345072 -2.314232 -1.772990 -0.637345

 33 N3 NC S 4.441143 -0.450773 -0.879715 -0.898360

 34 C4 CA B 3.520346 0.142266 -0.228935 1.143367

 35 C5 CM S 2.412205 -0.696628 0.264935 -0.749415

 36 H5 HA E 1.608484 -0.252222 0.853846 0.229665

 37 N4 N2 B 3.536914 1.422858 -0.000002 -1.143603

 38 H41 H E 4.317481 1.999065 -0.342843 0.467716

 39 H42 H E 2.767936 1.872486 0.521085 0.467716

 40 C6 CM S 2.376671 -2.008005 0.006873 0.029107

 41 H6 H4 E 1.532950 -2.544424 0.425736 0.185208

 42 C3' CT M 2.204303 -6.219073 -0.559481 -0.103397

 43 H3' H1 E 1.351306 -6.628587 0.007356 0.149381

 44 O3' OS M 2.976631 -7.427678 -0.785507 -0.465414

LOOP

 C2' C3'

 C5 C6

IMPROPER

DONE

STOP

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UMS.prepi:

0 0 0

 leap-generated prep residue

UMS.res

UMS INT 0

CHANGE NOMIT DU BEG

 0.00000

 1 DUMM DU M 0.000000 0.000000 0.000000 0.0

 2 DUMM DU M 1.000000 0.000000 0.000000 0.0

 3 DUMM DU M 1.000000 1.000000 0.000000 0.0

 4 P P M -1.647371 -3.674938 0.169036 0.807190

 5 O1P O2 E -1.394666 -2.957248 1.452440 -0.691354

 6 SP SH E -2.687606 -4.718069 0.348043 -0.160369

 7 O5' OS M -0.299145 -4.314426 -0.399954 -0.170826

 8 C5' CT M -0.116233 -4.800063 -1.738907 -0.445811

 9 H5'1 H1 E -0.279746 -4.004279 -2.482003 0.162101

 10 H5'2 H1 E -0.865096 -5.585810 -1.910975 0.162101

 11 C4' CT M 1.316581 -5.360284 -1.935881 0.606004

 12 H4' H1 E 1.321890 -6.059247 -2.787836 0.029509

 13 O4' OS S 2.153725 -4.223339 -2.228983 -0.595782

 14 C1' CT 3 2.939074 -3.881872 -1.080020 0.128649

 15 H1' H2 E 3.919764 -4.263029 -1.376020 0.140178

 16 C2' CT B 2.469562 -4.813544 0.081255 0.315610

 17 H2'1 H1 E 1.741551 -4.380771 0.778476 -0.019944

 18 O2' OS S 3.563385 -5.206534 0.888308 -0.343676

 19 C10 CT 3 4.199174 -4.124698 1.574095 0.138581

 20 H101 H1 E 3.783194 -4.053511 2.587751 0.033708

 21 H102 H1 E 4.163324 -3.128010 1.117219 0.033708

 22 C11 CT 3 5.667016 -4.564960 1.505080 -0.073057

 23 H111 H1 E 6.295879 -3.820497 2.015283 0.079208

 24 H112 H1 E 5.755824 -5.543474 2.001894 0.079208

 25 O11 OS S 6.008264 -4.682325 0.107931 -0.237370

 26 C12 CT 3 7.376661 -5.063690 -0.088046 -0.178225

 27 H121 H1 E 7.576902 -5.171323 -1.164298 0.102085

 28 H122 H1 E 7.585437 -6.023206 0.409893 0.102085

 29 H123 H1 E 8.033167 -4.280510 0.318930 0.102085

 30 N1 N\* B 3.090340 -2.435819 -0.820058 0.064936

 31 C2 C B 4.211132 -1.772108 -1.244177 0.742559

 32 O2 O E 5.096411 -2.324568 -1.872344 -0.625232

 33 N3 NA B 4.360652 -0.456711 -0.946142 -0.698017

 34 H3 H E 5.190509 0.024732 -1.242057 0.406398

 35 C4 C B 3.433163 0.231675 -0.257002 0.888700

 36 O4 O E 3.536914 1.422858 -0.000002 -0.643673

 37 C5 CM S 2.250938 -0.497306 0.205843 -0.588601

 38 H5 HA E 1.482206 0.010099 0.788675 0.246478

 39 C6 CM S 2.143355 -1.795751 -0.094216 -0.062709

 40 H6 H4 E 1.257982 -2.290581 0.293924 0.184738

 41 C3' CT M 1.823955 -6.028497 -0.632592 -0.128958

 42 H3' H1 E 0.967064 -6.413933 -0.054850 0.160325

 43 O3' OS M 2.557290 -7.265151 -0.835599 -0.458037

LOOP

 C2' C3'

 C5 C6

IMPROPER

DONE

STOP

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