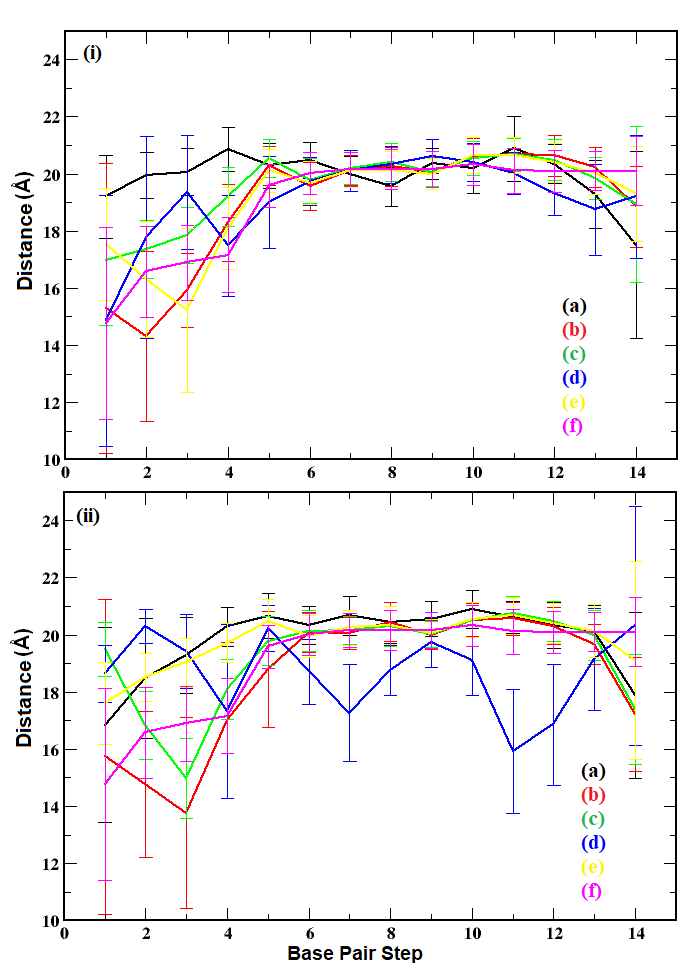
**Supplementary Information**



**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 ± 22.95  24.62 ± 21.90  10.69 ± 20.10 | 33.04 ± 12.11  26.80 ± 7.99  32.21 ± 13.89 |
| **b** | -2.98 ± 1.86  -3.27 ± 2.37  -4.69 ± 3.85 | 11.88 ± 15.46  12.73 ± 8.98  13.71 ± 16.88 | 30.25 ± 8.31  32.15 ± 3.23  28.16 ± 7.91 |
| **c** | -4.21 ± 1.31  -3.97 ± 2.78  -4.15 ± 2.16 | 13.21 *±* 14.97  17.15 ± 19.08  9.79 ± 11.05 | 33.27 ± 7.79  34.29 ± 10.52  30.65 ± 5.96 |
| **d** | -5.00 ± 1.13  -2.01 ± 2.14  -4.44 ± 3.64 | 34.05 ± 10.92  7.83 ± 17.86  22.57 ± 25.02 | 36.78 ± 2.94  1.66 ± 84.60  39.63 ± 20.76 |
| **e** | -4.78 ± 1.64  -5.30 ± 5.70  -3.60 ± 2.59 | 20.31 ± 18.45  5.08 ± 10.88  3.49 ± 15.64 | 31.84 ± 7.92  28.00 ± 8.34  31.49 ± 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-G  T-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  T-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-G  U-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  U-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-G  U-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  U-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-G  U-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  U-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-G  U-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  U-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-G  U-A  T-A  A-T  G-C  C-G  A-T  C-G  T-A  G-C  G-C C-G  C-G  U-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-A  T-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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-A  U-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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-A  U-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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-A  U-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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-A  U-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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-A  U-A/ T-A  T-A/ A-T  A-T/ G-C  G-C/ C-G  C-G/ A-T  A-T/ C-G  C-G/ T-A  T-A/ G-C  G-C/ G-C  G-C/ C-G C-G/ C-G  C-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** | 82.45  44.43  43.44  42.94  41.12  ---  --- | | 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** | 94.62  47.22  43.34  --- | | ---  ---  51.90  55.01 | | ---  ---  ---  --- | | 53.17  ---  ---  --- | | ---  ---  ---  --- | | ---  ---  ---  --- |
| **3T:A26** | | **N3-H3---N1**  **O4---H62-N6**  **O4---H61-N6** | 98.06  46.71  43.17 | | 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  ---  --- | | ---  62.15  53.95 | | ---  ---  --- | | ---  ---  --- | | ---  ---  --- |
| **3T:G28** | | **O2---H1-N1** | --- | | --- | | 48.76 | | --- | | --- | | --- |
| **4A:U25** | | **N1---H3-N3**  **N6-H62---O4**  **N6-H61---O4** | 96.99  46.45  45.61 | | 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** | 98.17  50.66  47.89  46.33  46.18 | | 99.99  ---  99.99  99.15  --- | | 99.89  ---  99.90  99.02  --- | | 74.90  45.67  40.69  ---  --- | | 99.97  ---  99.94  99.30  --- | | 99.93  ---  99.80  98.73  --- |
| **6C:G23** | | **N3---H1-N1**  **O2---H21-N2**  **N4-H41---O6**  **O2---H22-N2**  **O2---H1-N1** | 99.45  51.76  48.32  46.88  --- | | 99.95  99.99  99.64  ---  --- | | 99.98  99.99  99.58  ---  40.20 | | 99.32  44.63  44.57  53.40  44.03 | | 99.97  99.97  99.65  ---  40.89 | | 99.90  99.99  99.04  ---  --- |
| **7A:U22** | | **N1---H3-N3**  **N6-H62---O4**  **N6-H61---O4** | 99.53  47.98  45.82 | | 99.79  ---  96.52 | | 99.82  ---  96.20 | | 98.00  41.94  48.55 | | 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** | 97.79  60.85  50.90  48.00  45.63 | | 100.00  47.27  ---  99.54  99.99 | | 99.98  47.93  ---  99.61  100.00 | | 99.54  54.99  48.14  46.81  49.50 | | 99.99  48.13  ---  99.66  99.99 | | 99.74  ---  ---  99.26  99.96 |
| **9T:A20** | | **N3-H3---N1**  **O4---H62-N6**  **O4---H61-N6** | 99.10  47.96  47.89 | | 99.95  ---  98.02 | | 99.97  ---  98.08 | | 99.29  49.03  46.26 | | 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** | 97.45  50.21  47.17  47.10  47.03 | | 99.97  ---  ---  99.70  99.98 | | 99.90  ---  ---  99.56  99.98 | | 85.27  46.62  ---  42.51  43.39 | | 99.97  ---  ---  99.58  99.97 | | 99.87  ---  ---  99.37  99.94 |
| **11G:C18** | | **N1-H1---N3**  **N2-H22---O2**  **N2-H21---O2**  **O6---H41-N4**  **O6---H42-N4** | 95.60  50.06  45.86  45.46  44.24 | | 99.96  ---  99.99  99.38  --- | | 99.93  ---  100.00  99.49  --- | | 72.71  42.56  45.92  ---  --- | | 99.96  ---  99.99  99.39  --- | | 99.91  ---  99.97  99.06  --- |
| **12C:G17** | | **N3---H1-N1**  **O2---H21-N2**  **N4-H41---O6**  **O2---H22-N2**  **O2---H1-N1** | 99.66  51.74  51.14  47.07  44.43 | | 99.99  99.99  99.76  ---  --- | | 99.99  99.98  99.71  ---  --- | | 76.76  ---  ---  41.72  59.68 | | 99.99  100.00  99.47  ---  --- | | 99.99  100.00  99.50  ---  --- |
| **13C:G16** | | **N3---H1-N1**  **O2---H21-N2**  **O2---H22-N2**  **N4-H41---O6**  **O2---H1-N1** | 59.83  49.74  41.37  ---  --- | | 100.00  100.00  ---  99.75  --- | | ---  99.98  ---  ---  40.69 | | ---  ---  ---  ---  --- | | 100.00  ---  ---  47.30 | | 99.99  99.98  ---  99.59  --- |
| **14T:A15** | | **N3-H3---N1**  **O4---H61-N6** | ---  --- | | 53.12  50.90 | | ---  --- | | ---  --- | | ---  75.80 | | 87.37  84.46 |
| **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  ---  ---  45.85  44.75  47.24  46.59 | | ---  ---  ---  ---  ---  ---  --- | | ---  ---  ---  ---  ---  ---  --- | |
| **2T:A27** | **N3-H3---N1**  **O4---H61-N6**  **O4---H62-N6**  **N3-H3---N7** | | 51.11  ---  ---  --- | ---  ---  ---  --- | | ---  ---  69.75  --- | | 96.19  41.46  40.84  --- | | ---  48.85  ---  --- | | ---  ---  ---  --- | |
| **2T:G28** | **O2---H1-N1** | | --- | --- | | --- | | --- | | 52.94 | | --- | |
| **3T:A26** | **N3-H3---N1**  **O4---H62-N6**  **O4---H61-N6** | | 96.38  40.84  44.49 | ---  ---  --- | | 92.39  ---  86.84 | | 95.11  43.03  46.28 | | 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** | | 96.43  45.80  47.26 | 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** | | 97.23  48.93  49.51  49.11  42.93 | 99.77  ---  99.92  97.41  --- | | 99.90  ---  99.90  98.59  --- | | 87.25  47.71  42.12  42.67  42.72 | | 99.94  ---  99.98  98.74 | | 99.93  ---  99.80  98.73  --- | |
| **6C:G23** | **N3---H1-N1**  **O2---H21-N2**  **N4-H41---O6**  **O2---H22-N2**  **O2---H1-N1** | | 99.56  48.41  47.98  49.79  40.03 | 99.97  99.93  99.65  --- | | 99.95  99.99  99.49  ---  40.89 | | 99.50  45.52  47.56  51.01  54.27 | | 99.98  99.99  99.60  ---  --- | | 99.90  99.99  99.04  ---  --- | |
| **7A:U22** | **N1---H3-N3**  **N6-H62---O4**  **N6-H61---O4** | | 99.54  42.01  53.43 | 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** | | 99.13  50.55  47.41  48.56  50.64 | 99.91  49.55  ---  99.58  99.98 | | 99.99  48.19  ---  99.68  100.00 | | 92.57  48.40  49.71  41.62  --- | | 99.98  46.51  ---  99.60  99.99 | | 99.74  ---  ---  99.26  99.96 | |
| **9T:A20** | **N3-H3---N1**  **O4---H62-N6**  **O4---H61-N6** | | 99.53  46.11  47.13 | 99.98  ---  97.16 | | 99.97  ---  97.23 | | 94.34  46.55  40.61 | | 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** | | 97.28  49.34  46.49  46.92  45.87 | 99.97  ---  ---  99.60  99.99 | | 99.74  ---  ---  99.50  100.00 | | 68.60  41.28  ---  ---  41.30 | | 99.79  ---  ---  99.48  99.99 | | 99.87  ---  ---  99.37  99.94 | |
| **11G:C18** | **N1-H1---N3**  **N2-H22---O2**  **N2-H21---O2**  **O6---H41-N4**  **O6---H42-N4** | | 89.43  48.66  47.15  41.01  41.94 | 99.82  ---  99.98  99.22  --- | | 99.86  ---  99.99  99.24  --- | | ---  ---  ---  ---  --- | | 99.98  ---  100.00  99.41  --- | | 99.91  ---  99.97  99.06  --- | |
| **12C:G17** | **N3---H1-N1**  **O2---H21-N2**  **N4-H41---O6**  **O2---H22-N2**  **O2---H1-N1** | | 99.70  50.82  49.36  48.16  40.09 | 99.96  99.99  99.65  ---  --- | | 100.00  100.00  99.73  ---  --- | | 83.12  41.49  46.83  43.03  51.27 | | 99.93  100.00  99.44  ---  --- | | 99.99  100.00  99.50  ---  --- | |
| **13C:G16** | **N3---H1-N1**  **O2---H21-N2**  **O2---H22-N2**  **N4-H41---O6**  **N4-H42---O6**  **O2---H1-N1** | | 98.79  52.45  45.91  49.17  47.89  41.30 | 100.00  99.97  ---  99.81  ---  42.38 | | ---  99.94  ---  ---  ---  --- | | 46.89  99.85  ---  ---  ---  49.47 | | ---  ---  ---  ---  ---  --- | | 99.99  99.98  ---  99.59  ---  --- | |
| **14T:A15** | **N3-H3---N1**  **O4---H61-N6**  **O2---H62-N6** | | 60.69  ---  --- | ---  ---  63.23 | | ---  ---  --- | | ---  ---  --- | | ---  ---  --- | | 87.37  84.46  --- | |
| **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

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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

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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

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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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