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Supplemental Information

DHHC20 Palmitoyl-Transferase Reshapes the Membrane to Foster Catalysis

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Palmitoyl-CoA topology

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RESI PCA        -4.00

GROUP
ATOM CG  CT3 -0.27 !                HG3
ATOM HG1 HA3  0.09 !                 |
ATOM HG2 HA3  0.09 !              HG2--CG--HG1
ATOM HG3 HA3  0.09 !                 |

GROUP
ATOM CF  CT2 -0.18 !              HF2--CF--HF1
ATOM HF1 HA2  0.09 !                 |
ATOM HF2 HA2  0.09

GROUP
ATOM CE  CT2 -0.18 !              HE2--CE--HE1
ATOM HE1 HA2  0.09 !                 |
ATOM HE2 HA2  0.09

GROUP
ATOM CD  CT2 -0.18 !              HD2--CD--HD1
ATOM HD1 HA2  0.09 !                 |
ATOM HD2 HA2  0.09

GROUP
ATOM CC  CT2 -0.18 !              HC2--CC--HC1
ATOM HC1 HA2  0.09 !                 |
ATOM HC2 HA2  0.09

GROUP
ATOM CB  CT2 -0.18 !              HB2--CB--HB1
ATOM HB1 HA2  0.09 !                 |
ATOM HB2 HA2  0.09

GROUP
ATOM CA  CT2 -0.18 !              HA2--CA--HA1
ATOM HA1 HA2  0.09 !                 |
ATOM HA2 HA2  0.09
```

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GROUP
ATOM C9  CT2 -0.18 !            H92--C9--H91
ATOM H91 HA2  0.09 !                 |
ATOM H92 HA2  0.09

GROUP
ATOM C8  CT2 -0.18 !            H82--C8--H81
ATOM H81 HA2  0.09 !                 |
ATOM H82 HA2  0.09

GROUP
ATOM C7   CT2 -0.18 !           H72--C7--H71
ATOM H71  HA2  0.09 !                |
ATOM H72  HA2  0.09

GROUP
ATOM C6   CT2 -0.18 !           H62--C6--H61
ATOM H61  HA2  0.09 !                |
ATOM H62  HA2  0.09

GROUP
ATOM C5   CT2 -0.18 !           H51--C5--H52
ATOM H51  HA2  0.09 !                |
ATOM H52  HA2  0.09

GROUP
ATOM C4   CT2 -0.18 !           H42--C4--H41
ATOM H41  HA2  0.09 !                |
ATOM H42  HA2  0.09

GROUP
ATOM C3   CT2 -0.18 !           H32--C3--H31
ATOM H31  HA2    0.09 !              |
ATOM H32  HA2    0.09

GROUP
ATOM C2   CT2          -0.18 !  H2 --C2--H1   H21
ATOM H1   HA2           0.09 !      |        |
ATOM H2   HA2           0.09 !      C1--S1P--C2P--
ATOM C1    C            0.44 !     //        |
ATOM O2    O           -0.39 !     O2        H22
ATOM S1P   S           -0.09
ATOM C2P   CT2         -0.14
ATOM H21   HA2          0.09
ATOM H22   HA2          0.09
```

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GROUP
ATOM C3P   CT2        -0.02 !  H3X       O5P  H6X
ATOM H3X   HA2         0.09 !   |        ||   |
ATOM H3Y   HA2         0.09 !--C3P--N4P--C5P--C6P--
ATOM N4P   NH1        -0.47 !   |    |        |
ATOM HN4   H           0.31 !  H3Y  HN4       H6Y

GROUP
ATOM C5P   C           0.51
ATOM O5P   O          -0.51

GROUP
ATOM C6P   CT2        -0.18
ATOM H6X   HA2         0.09
ATOM H6Y   HA2         0.09

GROUP
ATOM C7P   CT2        -0.02 !  H7X       O9P
ATOM H7X   HA2         0.09 !   |        ||
ATOM H7Y   HA2         0.09 !--C7P--N8P--C9P--
ATOM N8P   NH1        -0.47 !   |    |
ATOM HN8   H           0.31 !  H7Y  HN8

GROUP
ATOM C9P   C           0.51
ATOM O9P   O          -0.51

GROUP
ATOM CAP   CT1         0.14 !  H10  CEP(H3)
ATOM OAP   OH1        -0.66 !   |    |
ATOM HO1   H           0.43 !--CAP--CBP
ATOM H10   HA1         0.09 !   |    |
                     !  OAP  CDP(H3)
GROUP                !   |
ATOM CBP   CT1         0.00 !  HO1

GROUP
ATOM CEP   CT3        -0.27
ATOM H141  HA3         0.09
ATOM H142  HA3         0.09
ATOM H143  HA3         0.09

GROUP
ATOM CDP   CT3        -0.27
ATOM H131  HA3         0.09
ATOM H132  HA3         0.09
```

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ATOM H133  HA3          0.09

GROUP
ATOM CCP   CG321       -0.08 !  H121      05A
ATOM H121  HGA2         0.09 !   |         |
ATOM H122  HGA2         0.09 !--CCP--O6A--P2A--03A
ATOM O6A   OG303       -0.62 !   |         |
ATOM P2A   PG1          1.46 !  H122      04A
ATOM O5A   OG2P1       -0.83 !
ATOM O4A   OG2P1       -0.83 !
ATOM O3A   OG304       -0.63 !

GROUP
ATOM P1A   PG1          1.50 !    H61A   H62A
ATOM O1A   OG2P1       -0.82 !       \   /
ATOM O2A   OG2P1       -0.82 !        N6A
ATOM O5B   OG303       -0.61 !         |
ATOM C5B   CG321       -0.08 !        C6A
ATOM H51A  HGA2         0.09 !       //  \
ATOM H52A  HGA2         0.09 !      N1A  C5A--N7A
                        !     |     ||     \\
GROUP                   !     |     ||      C8A--H8A
ATOM C4B   CG3C51       0.16 !      |     ||      /
ATOM H4B   HGA1         0.09 !      C2A   C4A--N9A
ATOM O4B   OG3C51      -0.50 !     / \\   /     \
ATOM C1B   CG3C51       0.16 !   H2A   N3A       \
ATOM H1B   HGA1         0.09 !                    \
                        !                  \
GROUP                   !                   \
ATOM N9A   NG2R51      -0.05 !                     \
ATOM C5A   CG2RC0       0.28 ! O1A      H51A H4B  04B \
ATOM N7A   NG2R50      -0.71 !  |         |    \ /   \ \
ATOM C8A   CG2R53       0.34 !-P1A--05B--C5B--C4B     C1B
ATOM H8A   HGR52        0.12 !  |         |     \     / \
ATOM N1A   NG2R62      -0.74 ! O2A      H52A   C3B--C2B  H1B
ATOM C2A   CG2R64       0.50 !               / \   / \
ATOM H2A   HGR62        0.13 !             03B H3B 02B H2B
ATOM N3A   NG2R62      -0.75 !              |       |
ATOM C4A   CG2RC0       0.43 !        O8A--P3B--O7A  H02A
ATOM C6A   CG2R64       0.46 !             |
ATOM N6A   NG2S3       -0.77 !            O9A
ATOM H61A  HGP4         0.38
ATOM H62A  HGP4         0.38

GROUP
ATOM C2B   CG3C51       0.14
```

```
ATOM H2B   HGA1         0.09
ATOM O2B   OG311       -0.66
ATOM HO2A  HGP1         0.43

GROUP
ATOM C3B   CG3C51      -0.09
ATOM H3B   HGA1         0.09
ATOM P3B   PG2          1.10
ATOM O7A   OG2P1       -0.90
ATOM O8A   OG2P1       -0.90
ATOM O3B   OG303       -0.40
ATOM O9A   OG2P1       -0.90

BOND   CG   HG1  CG   HG2  CG   HG3
BOND   CF   CG   CF   HF1  CF   HF2
BOND   CE   CF   CE   HE1  CE   HE2
BOND   CD   CE   CD   HD1  CD   HD2
BOND   CC   CD   CC   HC1  CC   HC2
BOND   CB   CC   CB   HB1  CB   HB2
BOND   CA   CB   CA   HA1  CA   HA2
BOND   C9   CA   C9   H91  C9   H92
BOND   C8   C9   C8   H81  C8   H82
BOND   C7   C8   C7   H71  C7   H72
BOND   C6   C7   C6   H61  C6   H62
BOND   C5   C6   C5   H51  C5   H52
BOND   C4   C5   C4   H41  C4   H42
BOND   C3   C4   C3   H31  C3   H32
BOND   C2   H1   C2   H2   C2   C3
BOND   C2   C1   C1   O2   S1P  C1
BOND   C2P  S1P  C2P  H21  C2P  H22
BOND   C2P  C3P
BOND   C3P  H3X  C3P  H3Y  C3P  N4P
BOND   N4P  HN4  N4P  C5P
BOND   C5P  O5P  C5P  C6P
BOND   C6P  H6X  C6P  H6Y
BOND   C6P  C7P
BOND   C7P  H7X  C7P  H7Y  C7P  N8P
BOND   N8P  HN8  N8P  C9P
BOND   C9P  O9P
BOND   C9P  CAP
BOND   CAP  OAP  CAP  H10  CAP  CBP  OAP  HO1
BOND   CBP  CDP  CBP  CEP
BOND   CDP  H131 CDP  H132 CDP  H133
BOND   CEP  H141 CEP  H142 CEP  H143
BOND   CBP  CCP
BOND   P1A  O3A  O3A  P2A
```

```
BOND   P2A  O5A  P2A  O4A  P2A  O6A
BOND   O6A  CCP  CCP  H121 CCP  H122
BOND   P1A  O1A  P1A  O2A  P1A  O5B
BOND   O5B  C5B  C5B  C4B  C4B  O4B  C4B  C3B  O4B  C1B
BOND   C1B  N9A  C1B  C2B  N9A  C4A  N9A  C8A  C4A  N3A
BOND   C2A  N1A  C6A  N6A
BOND   N6A  H61A N6A  H62A C6A  C5A  C5A  N7A
BOND   C2B  C3B  C2B  O2B  O2B  HO2A  C3B  O3B
BOND   C1B  H1B  C2B  H2B  C3B  H3B  C4B  H4B  C5B  H51A
BOND   C5B  H52A C8A  H8A  C2A  H2A
DOUBLE  N1A  C6A  C2A  N3A  C4A  C5A  N7A  C8A
BOND   O3B  P3B  P3B  O7A  P3B  O8A  P3B  O9A

IMPR   C1   S1P  C2   O2
IMPR   N4P  C5P  C3P  HN4
IMPR   C5P  C6P  N4P  O5P
IMPR   N8P  C9P  C7P  HN8
IMPR   C9P  CAP  N8P  O9P
IMPR   N6A  H61A H62A C6A
IMPR   C6A  C5A  N1A  N6A

END
RETURN
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Caprylic-CoA topology

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RESI CCOA     -4.00

GROUP
ATOM C8  CT3  -0.27
ATOM H81 HA3  0.09
ATOM H82 HA3  0.09
ATOM H83 HA3  0.09

GROUP
ATOM C7   CT2 -0.18
ATOM H71  HA2  0.09
ATOM H72  HA2  0.09

GROUP
ATOM C6   CT2 -0.18
ATOM H61  HA2  0.09
ATOM H62  HA2  0.09

GROUP
ATOM C5   CT2 -0.18
ATOM H51  HA2  0.09
ATOM H52  HA2  0.09

GROUP
ATOM C4   CT2 -0.18
ATOM H41  HA2  0.09
ATOM H42  HA2  0.09

GROUP
ATOM C3   CT2 -0.18
ATOM H31  HA2    0.09
ATOM H32  HA2    0.09

GROUP
ATOM C2   CT2          -0.18
ATOM H1   HA2           0.09
ATOM H2   HA2           0.09
ATOM C1    C           0.44
```

```
ATOM O2    O          -0.39
ATOM S1P   S          -0.09
ATOM C2P   CT2         -0.14
ATOM H21   HA2          0.09
ATOM H22   HA2          0.09

GROUP
ATOM C3P   CT2         -0.02
ATOM H3X   HA2          0.09
ATOM H3Y   HA2          0.09
ATOM N4P   NH1         -0.47
ATOM HN4   H           0.31

GROUP
ATOM C5P   C           0.51
ATOM O5P   O          -0.51

GROUP
ATOM C6P   CT2         -0.18
ATOM H6X   HA2          0.09
ATOM H6Y   HA2          0.09

GROUP
ATOM C7P   CT2         -0.02
ATOM H7X   HA2          0.09
ATOM H7Y   HA2          0.09
ATOM N8P   NH1         -0.47
ATOM HN8   H           0.31

GROUP
ATOM C9P   C           0.51
ATOM O9P   O          -0.51

GROUP
ATOM CAP   CT1          0.14
ATOM OAP   OH1         -0.66
ATOM HO1   H           0.43
ATOM H10   HA1          0.09

GROUP
ATOM CBP   CT1          0.00

GROUP
ATOM CEP   CT3         -0.27
ATOM H141  HA3          0.09
ATOM H142  HA3          0.09
```

```
ATOM H143  HA3          0.09

GROUP
ATOM CDP   CT3         -0.27
ATOM H131  HA3          0.09
ATOM H132  HA3          0.09
ATOM H133  HA3          0.09

GROUP
ATOM CCP   CG321       -0.08
ATOM H121  HGA2         0.09
ATOM H122  HGA2         0.09
ATOM O6A   OG303       -0.62
ATOM P2A   PG1          1.46
ATOM O5A   OG2P1       -0.83
ATOM O4A   OG2P1       -0.83
ATOM O3A   OG304       -0.63

GROUP
ATOM P1A   PG1          1.50
ATOM O1A   OG2P1       -0.82
ATOM O2A   OG2P1       -0.82
ATOM O5B   OG303       -0.61
ATOM C5B   CG321       -0.08
ATOM H51A  HGA2         0.09
ATOM H52A  HGA2         0.09

GROUP
ATOM C4B   CG3C51       0.16
ATOM H4B   HGA1         0.09
ATOM O4B   OG3C51      -0.50
ATOM C1B   CG3C51       0.16
ATOM H1B   HGA1         0.09

GROUP
ATOM N9A   NG2R51      -0.05
ATOM C5A   CG2RC0       0.28
ATOM N7A   NG2R50      -0.71
ATOM C8A   CG2R53       0.34
ATOM H8A   HGR52        0.12
ATOM N1A   NG2R62      -0.74
ATOM C2A   CG2R64       0.50
ATOM H2A   HGR62        0.13
ATOM N3A   NG2R62      -0.75
ATOM C4A   CG2RC0       0.43
ATOM C6A   CG2R64       0.46
```

```
ATOM N6A   NG2S3       -0.77
ATOM H61A  HGP4         0.38
ATOM H62A  HGP4         0.38

GROUP
ATOM C2B   CG3C51       0.14
ATOM H2B   HGA1         0.09
ATOM O2B   OG311        -0.66
ATOM HO2A  HGP1         0.43

GROUP
ATOM C3B   CG3C51      -0.09
ATOM H3B   HGA1         0.09
ATOM P3B   PG2          1.10
ATOM O7A   OG2P1        -0.90
ATOM O8A   OG2P1        -0.90
ATOM O3B   OG303        -0.40
ATOM O9A   OG2P1        -0.90

BOND   C8   H83  C8   H81  C8   H82
BOND   C7   C8   C7   H71  C7   H72
BOND   C6   C7   C6   H61  C6   H62
BOND   C5   C6   C5   H51  C5   H52
BOND   C4   C5   C4   H41  C4   H42
BOND   C3   C4   C3   H31  C3   H32
BOND   C2   H1   C2   H2   C2   C3
BOND   C2   C1   C1   O2   S1P  C1
BOND   C2P  S1P  C2P  H21  C2P  H22
BOND   C2P  C3P
BOND   C3P  H3X  C3P  H3Y  C3P  N4P
BOND   N4P  HN4  N4P  C5P
BOND   C5P  O5P  C5P  C6P
BOND   C6P  H6X  C6P  H6Y
BOND   C6P  C7P
BOND   C7P  H7X  C7P  H7Y  C7P  N8P
BOND   N8P  HN8  N8P  C9P
BOND   C9P  O9P
BOND   C9P  CAP
BOND   CAP  OAP  CAP  H10  CAP  CBP  OAP  HO1
BOND   CBP  CDP  CBP  CEP
BOND   CDP  H131 CDP  H132 CDP  H133
BOND   CEP  H141 CEP  H142 CEP  H143
BOND   CBP  CCP
BOND   P1A  O3A  O3A  P2A
BOND   P2A  O5A  P2A  O4A  P2A  O6A
BOND   O6A  CCP  CCP  H121 CCP  H122
```

```
BOND   P1A  O1A  P1A  O2A  P1A  O5B
BOND   O5B  C5B  C5B  C4B  C4B  O4B  C4B  C3B  O4B  C1B
BOND   C1B  N9A  C1B  C2B  N9A  C4A  N9A  C8A  C4A  N3A
BOND   C2A  N1A  C6A  N6A
BOND   N6A  H61A N6A  H62A C6A  C5A  C5A  N7A
BOND   C2B  C3B  C2B  O2B  O2B  HO2A  C3B  O3B
BOND   C1B  H1B  C2B  H2B  C3B  H3B  C4B  H4B  C5B  H51A
BOND   C5B  H52A C8A  H8A  C2A  H2A
DOUBLE  N1A  C6A  C2A  N3A  C4A  C5A  N7A  C8A
BOND   O3B  P3B  P3B  O7A  P3B  O8A  P3B  O9A
IMPR   C1   S1P  C2   O2
IMPR   N4P  C5P  C3P  HN4
IMPR   C5P  C6P  N4P  O5P
IMPR   N8P  C9P  C7P  HN8
IMPR   C9P  CAP  N8P  O9P
IMPR   N6A  H61A H62A C6A
IMPR   C6A  C5A  N1A  N6A
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Behenic-CoA topology

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RESI BCOA       -4.00

GROUP
ATOM CM  CT3 -0.27
ATOM HM1 HA3  0.09
ATOM HM2 HA3  0.09
ATOM HM3 HA3  0.09

GROUP
ATOM CL  CT2 -0.18
ATOM HL1 HA2  0.09
ATOM HL2 HA2  0.09

GROUP
ATOM CK  CT2 -0.18
ATOM HK1 HA2  0.09
ATOM HK2 HA2  0.09

GROUP
ATOM CJ  CT2 -0.18
ATOM HJ1 HA2  0.09
ATOM HJ2 HA2  0.09

GROUP
ATOM CI  CT2 -0.18
ATOM HI1 HA2  0.09
ATOM HI2 HA2  0.09

GROUP
ATOM CH  CT2 -0.18
ATOM HH1 HA2  0.09
ATOM HH2 HA2  0.09

GROUP
ATOM CG  CT2 -0.18
ATOM HG1 HA2  0.09
ATOM HG2 HA2  0.09
```

```
GROUP
ATOM CF  CT2 -0.18
ATOM HF1 HA2  0.09
ATOM HF2 HA2  0.09

GROUP
ATOM CE  CT2 -0.18
ATOM HE1 HA2  0.09
ATOM HE2 HA2  0.09

GROUP
ATOM CD  CT2 -0.18
ATOM HD1 HA2  0.09
ATOM HD2 HA2  0.09

GROUP
ATOM CC  CT2 -0.18
ATOM HC1 HA2  0.09
ATOM HC2 HA2  0.09

GROUP
ATOM CB  CT2 -0.18
ATOM HB1 HA2  0.09
ATOM HB2 HA2  0.09

GROUP
ATOM CA  CT2 -0.18
ATOM HA1 HA2  0.09
ATOM HA2 HA2  0.09

GROUP
ATOM C9  CT2 -0.18
ATOM H91 HA2  0.09
ATOM H92 HA2  0.09

GROUP
ATOM C8  CT2 -0.18
ATOM H81 HA2  0.09
ATOM H82 HA2  0.09

GROUP
ATOM C7   CT2 -0.18
ATOM H71  HA2  0.09
ATOM H72  HA2  0.09

GROUP
```

```
ATOM C6   CT2 -0.18
ATOM H61  HA2  0.09
ATOM H62  HA2  0.09

GROUP
ATOM C5   CT2 -0.18
ATOM H51  HA2  0.09
ATOM H52  HA2  0.09

GROUP
ATOM C4   CT2 -0.18
ATOM H41  HA2  0.09
ATOM H42  HA2  0.09

GROUP
ATOM C3   CT2 -0.18
ATOM H31  HA2    0.09
ATOM H32  HA2    0.09

GROUP
ATOM C2   CT2          -0.18
ATOM H1   HA2           0.09
ATOM H2   HA2           0.09
ATOM C1    C           0.44
ATOM O2    O          -0.39
ATOM S1P   S          -0.09
ATOM C2P   CT2         -0.14
ATOM H21   HA2          0.09
ATOM H22   HA2          0.09


GROUP
ATOM C3P   CT2         -0.02
ATOM H3X   HA2          0.09
ATOM H3Y   HA2          0.09
ATOM N4P   NH1         -0.47
ATOM HN4   H           0.31

GROUP
ATOM C5P   C           0.51
ATOM O5P   O          -0.51

GROUP
ATOM C6P   CT2         -0.18
ATOM H6X   HA2          0.09
ATOM H6Y   HA2          0.09
```

```
GROUP
ATOM C7P   CT2        -0.02
ATOM H7X   HA2         0.09
ATOM H7Y   HA2         0.09
ATOM N8P   NH1        -0.47
ATOM HN8   H          0.31

GROUP
ATOM C9P   C          0.51
ATOM O9P   O         -0.51

GROUP
ATOM CAP   CT1         0.14
ATOM OAP   OH1        -0.66
ATOM HO1   H          0.43
ATOM H10   HA1         0.09

GROUP
ATOM CBP   CT1         0.00

GROUP
ATOM CEP   CT3        -0.27
ATOM H141  HA3         0.09
ATOM H142  HA3         0.09
ATOM H143  HA3         0.09

GROUP
ATOM CDP   CT3        -0.27
ATOM H131  HA3         0.09
ATOM H132  HA3         0.09
ATOM H133  HA3         0.09

GROUP
ATOM CCP   CG321      -0.08
ATOM H121  HGA2        0.09
ATOM H122  HGA2        0.09
ATOM O6A   OG303      -0.62
ATOM P2A   PG1         1.46
ATOM O5A   OG2P1      -0.83
ATOM O4A   OG2P1      -0.83
ATOM O3A   OG304      -0.63

GROUP
ATOM P1A   PG1         1.50
ATOM O1A   OG2P1      -0.82
```

```
ATOM O2A   OG2P1       -0.82
ATOM O5B   OG303       -0.61
ATOM C5B   CG321       -0.08
ATOM H51A  HGA2         0.09
ATOM H52A  HGA2         0.09

GROUP
ATOM C4B   CG3C51       0.16
ATOM H4B   HGA1        0.09
ATOM O4B   OG3C51      -0.50
ATOM C1B   CG3C51       0.16
ATOM H1B   HGA1        0.09

GROUP
ATOM N9A   NG2R51      -0.05
ATOM C5A   CG2RC0       0.28
ATOM N7A   NG2R50      -0.71
ATOM C8A   CG2R53       0.34
ATOM H8A   HGR52        0.12
ATOM N1A   NG2R62      -0.74
ATOM C2A   CG2R64       0.50
ATOM H2A   HGR62        0.13
ATOM N3A   NG2R62      -0.75
ATOM C4A   CG2RC0       0.43
ATOM C6A   CG2R64       0.46
ATOM N6A   NG2S3       -0.77
ATOM H61A  HGP4         0.38
ATOM H62A  HGP4         0.38

GROUP
ATOM C2B   CG3C51       0.14
ATOM H2B   HGA1        0.09
ATOM O2B   OG311       -0.66
ATOM HO2A  HGP1         0.43

GROUP
ATOM C3B   CG3C51      -0.09
ATOM H3B   HGA1        0.09
ATOM P3B   PG2         1.10
ATOM O7A   OG2P1       -0.90
ATOM O8A   OG2P1       -0.90
ATOM O3B   OG303       -0.40
ATOM O9A   OG2P1       -0.90

BOND   CM   HM1  CM   HM2  CM   HM3
BOND   CL   CM   CL   HL1  CL   HL2
```

```
BOND   CK   CL   CK   HK1  CK   HK2
BOND   CJ   CK   CJ   HJ1  CJ   HJ2
BOND   CI   CJ   CI   HI1  CI   HI2
BOND   CH   CI   CH   HH1  CH   HH2
BOND   CG   CH   CG   HG1  CG   HG2
BOND   CF   CG   CF   HF1  CF   HF2
BOND   CE   CF   CE   HE1  CE   HE2
BOND   CD   CE   CD   HD1  CD   HD2
BOND   CC   CD   CC   HC1  CC   HC2
BOND   CB   CC   CB   HB1  CB   HB2
BOND   CA   CB   CA   HA1  CA   HA2
BOND   C9   CA   C9   H91  C9   H92
BOND   C8   C9   C8   H81  C8   H82
BOND   C7   C8   C7   H71  C7   H72
BOND   C6   C7   C6   H61  C6   H62
BOND   C5   C6   C5   H51  C5   H52
BOND   C4   C5   C4   H41  C4   H42
BOND   C3   C4   C3   H31  C3   H32
BOND   C2   H1   C2   H2   C2   C3
BOND   C2   C1   C1   O2   S1P  C1
BOND   C2P  S1P  C2P  H21  C2P  H22
BOND   C2P  C3P
BOND   C3P  H3X  C3P  H3Y  C3P  N4P
BOND   N4P  HN4  N4P  C5P
BOND   C5P  O5P  C5P  C6P
BOND   C6P  H6X  C6P  H6Y
BOND   C6P  C7P
BOND   C7P  H7X  C7P  H7Y  C7P  N8P
BOND   N8P  HN8  N8P  C9P
BOND   C9P  O9P
BOND   C9P  CAP
BOND   CAP  OAP  CAP  H10  CAP  CBP  OAP  HO1
BOND   CBP  CDP  CBP  CEP
BOND   CDP  H131 CDP  H132 CDP  H133
BOND   CEP  H141 CEP  H142 CEP  H143
BOND   CBP  CCP
BOND   P1A  O3A  O3A  P2A
BOND   P2A  O5A  P2A  O4A  P2A  O6A
BOND   O6A  CCP  CCP  H121 CCP  H122
BOND   P1A  O1A  P1A  O2A  P1A  O5B
BOND   O5B  C5B  C5B  C4B  C4B  O4B  C4B  C3B  O4B  C1B
BOND   C1B  N9A  C1B  C2B  N9A  C4A  N9A  C8A  C4A  N3A
BOND   C2A  N1A  C6A  N6A
BOND   N6A  H61A N6A  H62A C6A  C5A  C5A  N7A
BOND   C2A  N1A  C6A  N6A
BOND   N6A  H61A N6A  H62A C6A  C5A  C5A  N7A
```

```
BOND   C2B  C3B  C2B  O2B  O2B  HO2A  C3B  O3B
BOND   C1B  H1B  C2B  H2B  C3B  H3B  C4B  H4B  C5B  H51A
BOND   C5B  H52A C8A  H8A  C2A  H2A
DOUBLE  N1A  C6A  C2A  N3A  C4A  C5A  N7A  C8A
BOND   O3B  P3B  P3B  O7A  P3B  O8A  P3B  O9A
IMPR   C1   S1P  C2   O2
IMPR   N4P  C5P  C3P  HN4
IMPR   C5P  C6P  N4P  O5P
IMPR   N8P  C9P  C7P  HN8
IMPR   C9P  CAP  N8P  O9P
IMPR   N6A  H61A H62A C6A
IMPR   C6A  C5A  N1A  N6A

END
RETURN
```

Palmitoyl-CoA, Caprylic-CoA and Behenic-CoA parameters

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read param card flex append
*

BONDS
S   C              198.00  1.8180  ! Aleksandrov & Field (AAMF), Phys Chem Chem Phys 2011
CG321  CT1         222.50  1.5380  ! from CHARMM36 prot - modified from CT2 to CG321 (CH2 aliphatic carbon)

ANGLES
CT2   S     C              34.00  95.00                    ! AAMF
S     C     O              80.00  121.00                   ! AAMF
C     CT1   OH1            50.00  110.50                   ! AAMF
CT1   CG321 OG303          75.70  110.10                   ! from CHARMM36 cgenff - modified from CG311 to CT1 (both CH carbon)
CG321   CT1 CT1      53.35  111.00 8.00  2.5610    ! from CHARMM36 prot - modified from CT2 to CG321
CT3     CT1 CG321    53.35  114.00 8.00  2.5610    ! from CHARMM36 prot - modified from CT2 to CG321
HGA2  CG321 CT1      26.50  110.10 22.53 2.1790    ! from CHARMM36 prot - modified from CT2 to CG321 and HA2 to HGA2
S     C     CT2            50.00  114.00                   ! AAMF - modified from CT3 to CT2

DIHEDRALS
C   S   CT2 HA2          0.00         3 0.0  ! AAMF - modified from HA to HA2
HA2 CT2 C   S                0.04         3 0.0  ! AAMF - modified from CT3 to CT2, HA to HA2
CT2 CT2 C   S                0.24         1 180.0      ! based on AAMF
CT2 CT2 C   S                0.37         3 0.0  ! based on AAMF
C   S   CT2 CT2          0.24         1 180.0      ! AAMF
C   S   CT2 CT2          0.37         3 0.0  ! AAMF
O   C   S   CT2          3.73         1 180.0      ! AAMF
O   C   S   CT2          2.07         2 180.0      ! AAMF
CT2 C   S   CT2          2.63         1 180.0      ! AAMF - modified from CT3 to CT2
CT2 C   S   CT2          2.56         2 180.0      ! AAMF - modified from CT3 to CT2
NH1 C   CT2 CT2          2.98         1 0.0  ! AAMF
CT2 CT2 NH1 C                1.44         1 180.0      ! AAMF
CT2 CT2 NH1 C                0.30         3 180.0      ! AAMF
NH1 C   CT1 OH1          0.00         3 0.0  ! AAMF
O   C   CT1 OH1          0.00         3 0.0  ! AAMF
NH1 C   CT1 HA1          0.00         3 0.0  ! AAMF - modified from HA to HA1
O   C   CT1 HA1          0.00         3 0.0  ! AAMF - modified from HA to HA1
CT1 CT1  CG321  OG303        0.20         3 180.0      ! from CHARMM36 cgenff - modified from CG311 to CT1
CT1 CT1     CG321  HGA2      0.195 3 0.00         ! from CHARMM36 prot - modified from CT2 to CG321 and HA2 to HGA2
CT1 CG321  OG303  PG1        0.60         1 180.0      ! from CHARMM36 cgenff - modified from CG311 to CT1
CT1 CG321  OG303  PG1        0.65         2 0.00       ! from CHARMM36 cgenff - modified from CG311 to CT1
CT1 CG321  OG303  PG1        0.05         3 0.00       ! from CHARMM36 cgenff - modified from CG311 to CT1
CT3 CT1     CG321  OG303     0.20         3 180.0      ! from CHARMM36 cgenff - modified from CG311 to CT1 and CG331 to CT3
CT3 CT1  CG321  HGA2         0.195 1 0.00         ! from CHARMM36 prot - modified from CT2 to CG321 and HA2 to HGA2

END
RETURN
```