Supplementary Material (ESI) for PCCP

SUPPORTING INFORMATION.

Extension of the AMBER Force-Field for the Study of Large Nitroxides in Condensed Phases: An *ab initio* Parameterization.

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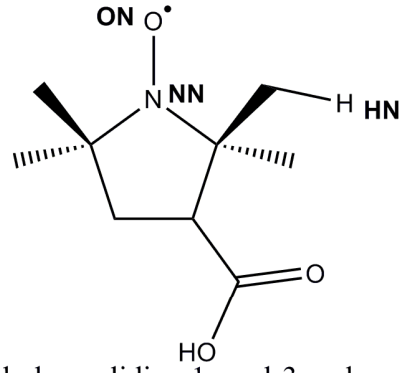
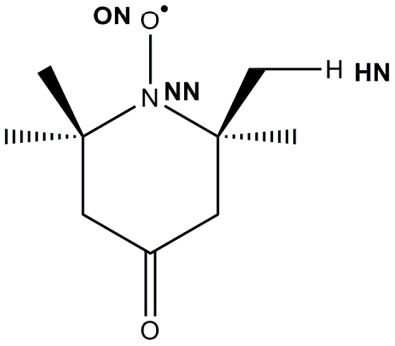
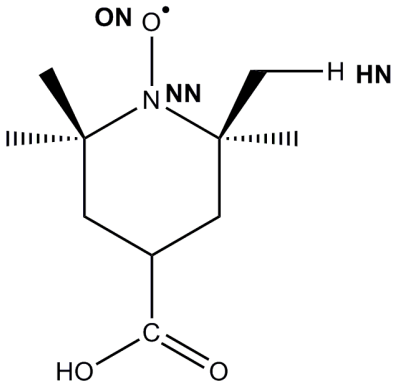
4 *Dipartimento di Chimica, Università di Modena e Reggio Emilia, Via G. Campi 183, 41100 Modena, ITALIA*



2,2,5,5-tetramethylpyrrolidine-1-oxyl-3-carboxylic acid
(3-carboxy-PROXYL)



4-oxo-2,2,6,6-tetramethylpiperidine-1-oxyl
(4-oxo-TEMPO)



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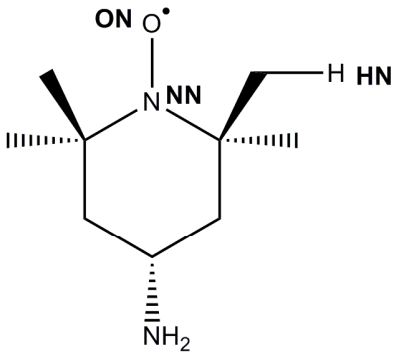
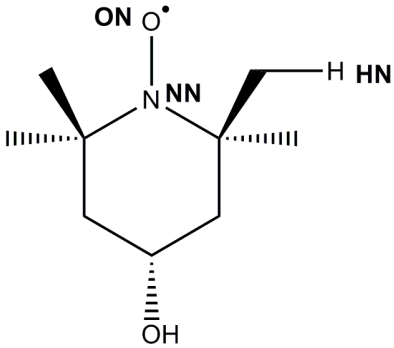
(4-carboxy-TEMPO)

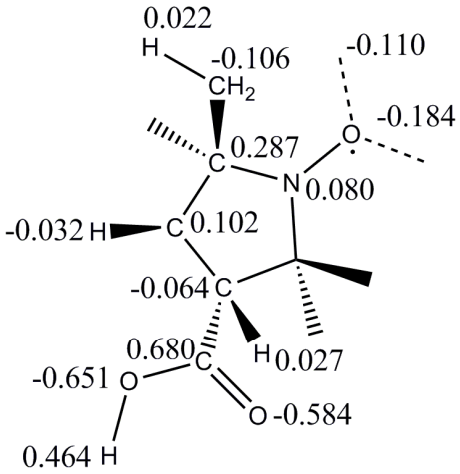


4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl
(TANINE)

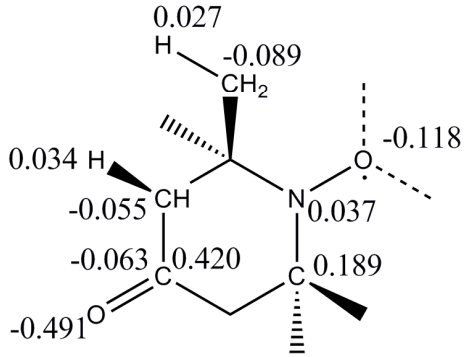


4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl
(TANOL)

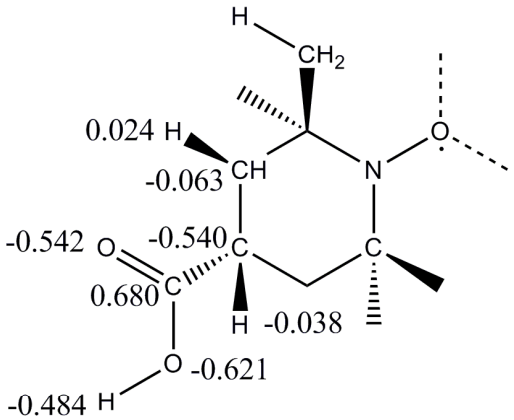
Figure S.1. Structures and atom types of other nitroxides considered in the present work



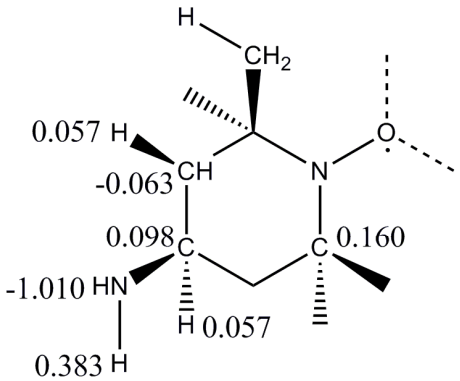
2,2,5,5-tetramethylpyrrolidine-1-oxyl-3-carboxylic acid
(3-carboxy-PROXYL)



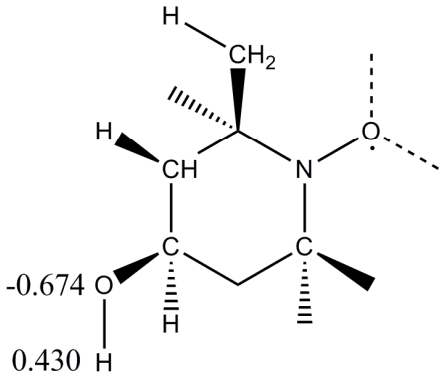
4-oxo-2,2,6,6-tetramethylpiperidine-1-oxyl
(4-oxo-TEMPO)



2,2,6,6-tetramethylpiperidine-1-oxyl-4-carboxylic acid
(4-carboxy-TEMPO)



4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl
(TANINE)



4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl
(TANOL)

Figure S.2. RESP charges of other nitroxides considered in the present work.

Table S.1. Structural features and nitrogen hyperfine coupling constants of 3-Oxo-PROXYL and NITNO.

	3-oxo-PROXYL		NITNO	
	QM	**MM**	**QM**	**MM**
Bond lengths (Å)				
N-O	1.260	1.260	1.259	1.256
N-C_2	1.486	1.483	1.345	1.345
Bond Angles (deg.)				
C_2-N-C_4	115.6	115.7	110.5	110.9
O-N-C_2	121.5	121.0	121.5	121.0
Regular torsions (deg.)				
O-N-C_2-C_3	174.1	171.2	180.0	179.0
C_5-N-C_2-C_3	8.3	8.1	-	-
Improper torsions (deg.)				
C_2-C_4-N-O	165.8	163.1	180.0	179.6
A_N (G)	13.0	13.0	6.8	6.9

frcmod.NITROXIDES.dat

```
Nitroxides parameters update of ff99SB (2009)

MASS
ON  16.00
NN  14.01
HN  1.008
CI  12.01
CE  12.01
CF  12.01
CX  12.01
CP  12.01
LP   9.00

BOND
ON-NN    360.00     1.258
CT-NN    370.00     1.477
CI-NN    370.00     1.485
CX-NN    370.00     1.340
CP-NN    370.00     1.477
CF-NN    428.00     1.390
CT-HN    340.00     1.090
C -CI    317.00     1.550
C -CP    317.00     1.522
CI-CA    317.00     1.510
CX-CT    317.00     1.455
CI-CT    310.00     1.526
CP-CT    310.00     1.526
C -CE    447.00     1.460
CF-CE    447.00     1.400
CF-CA    469.00     1.400
CE-CA    469.00     1.404
LP-ON    325.00     0.450

ANGLE
ON-NN-CT    82.00    117.50
ON-NN-CP    82.00    117.50
ON-NN-CF    82.00    121.50
ON-NN-CI    82.00    118.50
ON-NN-CX    82.00    120.00
CI-C -O     80.00    120.40
CP-C -O     80.00    120.40
CE-C -O     80.00    128.80
NN-CF-CA    70.00    132.80
C -CT-NN    70.00    108.70
CE-CF-NN    70.00    111.40
C -CI-NN    70.00    107.00
C -CP-NN    70.00    108.70
CA-CA-CI    70.00    120.00
C -CE-CA    63.00    134.90
NN-CT-CA    63.00    114.00
C -CI-CA    63.00    109.40
CT-CI-CA    63.00    112.00
CT-CI-C     63.00    111.10
CE-C -CT    63.00    106.40
CE-C -CI    63.00    106.40
C -CE-CF    63.00    108.00
NN-CI-CA    63.00    109.00
CF-CE-CA    63.00    116.20
```

```
CF-CA-CA    63.00    120.00
CE-CA-CA    63.00    120.00
CE-CF-CA    63.00    122.70
CT-CP-C     63.00    111.10
CP-C -CT    63.00    106.40
NN-CT-H1    61.12    106.30
CT-CT-NN    60.00    107.50
CT-CI-NN    60.00    107.50
CT-CP-NN    60.00    107.50
CT-NN-CT    52.60    120.80
CF-NN-CT    52.60    120.80
CP-NN-CT    52.60    120.80
CF-NN-CI    52.60    110.00
HN-CT-CT    50.00    109.50
HN-CT-CP    50.00    109.50
HC-CT-CI    50.00    109.50
CT-NN-CX    50.00    109.50
NN-CX-NN    50.00    109.00
NN-CX-CT    50.00    109.50
NT-CT-HP    50.00    109.50
CX-CT-HC    50.00    109.50
CE-CA-HA    50.00    120.00
CF-CA-HA    50.00    120.00
HN-CT-HN    35.00    109.50
CT-CP-CT    40.00    109.50
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LP-ON-LP    600.0    120.00

DIHEDRAL
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X -CF-NN-X      4   6.00    180.0  2
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X -CP-CT-X      9   1.40      0.0  3
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X -C -CI-X      6   0.00      0.0  2
X -C -CP-X      6   0.00      0.0  2
X -NN-CI-X      6   0.00      0.0  3
X -NN-CP-X      6   0.204     0.0  3
X -NN-CT-X      6   0.204     0.0  3
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X -C -CE-X      4  12.00    180.0  2
X -CA-CF-X      4  14.50    180.0  2
X -CE-CF-X      4  12.00    180.0  2
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ON-NN-CP-C      1   0.260     0.0  3
ON-NN-CP-CT     1   0.260     0.0  3
ON-NN-CT-H1     1   0.260     0.0  3
CT-NN-CT-H1     1   0.000     0.0  3
CT-NN-CT-CX     1   0.000     0.0  3
CT-NN-CP-C      1   0.000     0.0  3
CX-NN-CT-H1     1   0.100     0.0  3
NN-CT-CT-HN     1   0.100     0.0  3
NN-CT-CT-HC     1   0.100     0.0  3
NN-CX-CT-HC     1   0.100     0.0  3
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NN-CT-CT-CT     1   0.143     0.0  3
NN-CP -C-CT     1   0.000     0.0  2
HN-CT-CT-CT     1   0.160     0.0  3
CF-NN-CI-C      1   1.500   180.0  2
CE-C -CI-NN     1   1.500   180.0  2
C -CI-NN-ON     1   1.500   180.0  2
O -C -CI-NN     1   1.500   180.0  2
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IMPROPER TORSIONS
X -CT-NN-CX         1.10        180.          2.
CE-CI-C-O           1.10        180           2.
CA-CA-CA-CI         1.10        180.          2.
CF-CA-CE-C          1.10        180.          2.
CA-CE-CF-NN         1.10        180.          2.
LP-LP-ON-NN        10.10        180.          2.
NN-NN-CX-CT        10.10        180.          2.


NONBON
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NN      1.90    0.2627
ON      1.6750  0.2445
CF      1.9080  0.0860
CE      1.9080  0.0860
CI      1.9080  0.0860
CX      1.9080  0.0860
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LP      0.00    0.0000
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NITROXIDES09.lib

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 "O6" "ON" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "H11" "HN" 0 -1 0.0
 "H12" "HN" 0 -1 0.0
 "H13" "HN" 0 -1 0.0
 "H14" "HN" 0 -1 0.0
 "H15" "HN" 0 -1 0.0
 "H16" "HN" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HC" 0 -1 0.0
 "H24" "HC" 0 -1 0.0
 "H25" "HC" 0 -1 0.0
 "C26" "C" 0 -1 0.0
 "O27" "O2" 0 -1 0.0
 "O28" "O2" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.CPR.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.CPR.unit.childsequence single int
 2
!entry.CPR.unit.connect array int
```

```
 0
 0
!entry.CPR.unit.connectivity table  int atom1x  int atom2x  int flags
 1 9 1
 1 10 1
 1 5 1
 1 2 1
 2 3 1
 2 6 1
 3 4 1
 3 7 1
 3 8 1
 4 5 1
 4 24 1
 4 23 1
 5 26 1
 5 25 1
 6 29 1
 6 30 1
 7 12 1
 7 11 1
 7 13 1
 8 16 1
 8 14 1
 8 15 1
 9 17 1
 9 18 1
 9 19 1
 10 20 1
 10 21 1
 10 22 1
 26 28 1
 26 27 1
!entry.CPR.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
```

```
 "R" 1 "A" 29
 "R" 1 "A" 30
!entry.CPR.unit.name single str
 "3-CPROXYL"
!entry.CPR.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.483000
 1.342000 0.0 2.104000
 2.253000 -0.146000 0.880000
 1.459000 0.393000 -0.309000
 -1.055000 -0.076000 2.175000
 1.538000 1.334000 2.832000
 1.448000 -1.159000 3.091000
 -1.012000 1.006000 -0.527000
 -0.351000 -1.409000 -0.489000
 2.499000 1.342000 3.361000
 1.528000 2.168000 2.122000
 0.733000 1.487000 3.560000
 2.445000 -1.172000 3.547000
 0.695000 -1.061000 3.880000
 1.291000 -2.114000 2.578000
 -0.880000 1.071000 -1.611000
 -2.034000 0.699000 -0.280000
 -0.832000 1.996000 -0.091000
 -0.397000 -1.410000 -1.582000
 0.408000 -2.137000 -0.183000
 -1.321000 -1.710000 -0.076000
 3.203000 0.383000 1.012000
 2.501000 -1.195000 0.683000
 1.504000 1.491000 -0.326000
 1.942000 -0.093000 -1.714000
 2.865000 -0.934000 -1.725000
 1.324000 0.420000 -2.674000
 -1.456000 -0.105000 1.972000
 -1.030000 -0.074000 2.624000
!entry.CPR.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.CPR.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "CPR" 1 31 1 "?" 0
!entry.CPR.unit.residuesPdbSequenceNumber array int
 1
!entry.CPR.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.CPR.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```

```
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.CTH.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 0.037000
 "C2" "CT" 0 1 131074 2 6 0.189000
 "C3" "CT" 0 1 131074 3 6 -0.063000
 "C4" "CT" 0 1 131074 4 6 -0.054000
 "C5" "CT" 0 1 131074 5 6 -0.063000
 "C6" "CT" 0 1 131074 6 6 0.189000
 "C7" "CT" 0 1 131074 7 6 -0.089000
 "C8" "CT" 0 1 131074 8 6 -0.089000
 "C9" "CT" 0 1 131074 9 6 -0.089000
 "C10" "CT" 0 1 131074 10 6 -0.089000
 "O11" "ON" 0 1 131074 11 8 -0.118000
 "H12" "HC" 0 1 131074 12 1 0.038000
 "H13" "HC" 0 1 131074 13 1 0.024000
 "H14" "HC" 0 1 131074 14 1 0.024000
 "H15" "HC" 0 1 131074 15 1 0.024000
 "H16" "HC" 0 1 131074 16 1 0.024000
 "H17" "HN" 0 1 131074 17 1 0.027000
 "H18" "HN" 0 1 131074 18 1 0.027000
 "H19" "HN" 0 1 131074 19 1 0.027000
 "H20" "HN" 0 1 131074 20 1 0.027000
 "H21" "HN" 0 1 131074 21 1 0.027000
 "H22" "HN" 0 1 131074 22 1 0.027000
 "H23" "HN" 0 1 131074 23 1 0.027000
 "H24" "HN" 0 1 131074 24 1 0.027000
 "H25" "HN" 0 1 131074 25 1 0.027000
 "H26" "HN" 0 1 131074 26 1 0.027000
 "H27" "HN" 0 1 131074 27 1 0.027000
 "H28" "HN" 0 1 131074 28 1 0.027000
 "C29" "C" 0 1 131074 29 6 0.680100
 "O30" "O" 0 1 131074 30 8 -0.542100
 "O31" "OH" 0 1 131074 31 8 -0.621100
 "H32" "HO" 0 1 131074 32 1 0.484100
 "Lp1" "LP" 0 1 131074 33 0 -0.110000
 "Lp2" "LP" 0 1 131074 34 0 -0.110000
!entry.CTH.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
```

```
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "O11" "ON" 0 -1 0.0
 "H12" "HC" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HC" 0 -1 0.0
 "H16" "HC" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
 "H25" "HN" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "H27" "HN" 0 -1 0.0
 "H28" "HN" 0 -1 0.0
 "C29" "C" 0 -1 0.0
 "O30" "O" 0 -1 0.0
 "O31" "OH" 0 -1 0.0
 "H32" "HO" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.CTH.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.CTH.unit.childsequence single int
 2
!entry.CTH.unit.connect array int
 0
 0
!entry.CTH.unit.connectivity table  int atom1x  int atom2x  int flags
 1 6 1
 1 11 1
 1 2 1
 2 8 1
 2 7 1
 2 3 1
 3 4 1
 3 14 1
 3 13 1
 4 5 1
 4 12 1
 4 29 1
 5 6 1
 5 15 1
 5 16 1
 6 9 1
 6 10 1
 7 24 1
 7 23 1
 7 25 1
 8 27 1
 8 26 1
 8 28 1
 9 19 1
 9 18 1
```

```
 9 17 1
 10 22 1
 10 20 1
 10 21 1
 11 33 1
 11 34 1
 29 30 1
 29 31 1
 31 32 1
!entry.CTH.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
 "R" 1 "A" 33
 "R" 1 "A" 34
!entry.CTH.unit.name single str
 "4-CTEMPOH"
!entry.CTH.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.489000
 1.436000 0.0 2.023000
 2.343000 1.011000 1.323000
 2.386000 0.659000 -0.163000
 1.011000 0.702000 -0.838000
 -0.792000 1.213000 1.996000
 -0.698000 -1.282000 1.943000
 1.090000 -0.042000 -2.172000
 0.549000 2.144000 -1.090000
 -1.119000 -0.222000 -0.553000
 1.973000 2.032000 1.470000
 1.394000 0.192000 3.102000
 1.879000 -0.995000 1.893000
 3.050000 1.341000 -0.709000
```

```
 2.813000 -0.347000 -0.258000
 1.349000 -1.094000 -2.013000
 0.132000 0.002000 -2.695000
 1.861000 0.417000 -2.800000
 -0.477000 2.137000 -1.469000
 0.580000 2.759000 -0.186000
 1.195000 2.614000 -1.840000
 -0.282000 2.161000 1.798000
 -1.772000 1.239000 1.510000
 -0.942000 1.132000 3.079000
 -1.737000 -1.295000 1.607000
 -0.193000 -2.163000 1.534000
 -0.675000 -1.343000 3.036000
 3.734000 0.934000 1.904000
 4.427000 -0.053000 1.908000
 4.140000 2.104000 2.433000
 5.033000 1.954000 2.776000
 -1.485000 -0.295000 -0.301000
 -1.151000 -0.229000 -1.002000
!entry.CTH.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.CTH.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "CTH" 1 35 1 "?" 0
!entry.CTH.unit.residuesPdbSequenceNumber array int
 1
!entry.CTH.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.CTH.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```

```
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.CTM.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 0.037000
 "C2" "CT" 0 1 131074 2 6 0.189000
 "C3" "CT" 0 1 131074 3 6 -0.073000
 "C4" "CT" 0 1 131074 4 6 -0.105000
 "C5" "CT" 0 1 131074 5 6 -0.073000
 "C6" "CT" 0 1 131074 6 6 0.189000
 "C7" "CT" 0 1 131074 7 6 -0.089000
 "C8" "CT" 0 1 131074 8 6 -0.089000
 "C9" "CT" 0 1 131074 9 6 -0.089000
 "C10" "CT" 0 1 131074 10 6 -0.089000
 "O11" "ON" 0 1 131074 11 8 -0.118000
 "H12" "HC" 0 1 131074 12 1 0.034000
 "H13" "HC" 0 1 131074 13 1 0.024000
 "H14" "HC" 0 1 131074 14 1 0.024000
 "H15" "HC" 0 1 131074 15 1 0.024000
 "H16" "HC" 0 1 131074 16 1 0.024000
 "H17" "HN" 0 1 131074 17 1 0.027000
 "H18" "HN" 0 1 131074 18 1 0.027000
 "H19" "HN" 0 1 131074 19 1 0.027000
 "H20" "HN" 0 1 131074 20 1 0.027000
 "H21" "HN" 0 1 131074 21 1 0.027000
 "H22" "HN" 0 1 131074 22 1 0.027000
 "H23" "HN" 0 1 131074 23 1 0.027000
 "H24" "HN" 0 1 131074 24 1 0.027000
 "H25" "HN" 0 1 131074 25 1 0.027000
 "H26" "HN" 0 1 131074 26 1 0.027000
 "H27" "HN" 0 1 131074 27 1 0.027000
 "H28" "HN" 0 1 131074 28 1 0.027000
 "C29" "C" 0 1 131074 29 6 0.720000
 "O30" "O2" 0 1 131074 30 8 -0.822000
 "O31" "O2" 0 1 131074 31 8 -0.822000
 "Lp1" "LP" 0 1 131074 32 0 -0.110000
 "Lp2" "LP" 0 1 131074 33 0 -0.110000
!entry.CTM.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "O11" "ON" 0 -1 0.0
 "H12" "HC" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HC" 0 -1 0.0
 "H16" "HC" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
```

```
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
 "H25" "HN" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "H27" "HN" 0 -1 0.0
 "H28" "HN" 0 -1 0.0
 "C29" "C" 0 -1 0.0
 "O30" "O2" 0 -1 0.0
 "O31" "O2" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.CTM.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.CTM.unit.childsequence single int
 2
!entry.CTM.unit.connect array int
 0
 0
!entry.CTM.unit.connectivity table  int atom1x  int atom2x  int flags
 1 6 1
 1 11 1
 1 2 1
 2 8 1
 2 7 1
 2 3 1
 3 4 1
 3 14 1
 3 13 1
 4 5 1
 4 12 1
 4 29 1
 5 6 1
 5 15 1
 5 16 1
 6 9 1
 6 10 1
 7 24 1
 7 23 1
 7 25 1
 8 27 1
 8 26 1
 8 28 1
 9 19 1
 9 18 1
 9 17 1
 10 22 1
 10 20 1
 10 21 1
 11 32 1
 11 33 1
 29 30 1
 29 31 1
!entry.CTM.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
```

```
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
 "R" 1 "A" 33
!entry.CTM.unit.name single str
 "4-CTEMPO"
!entry.CTM.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.490000
 1.433000 0.0 2.033000
 2.377000 0.975000 1.346000
 2.408000 0.610000 -0.131000
 1.047000 0.655000 -0.834000
 -0.784000 1.226000 1.980000
 -0.722000 -1.271000 1.940000
 1.121000 -0.118000 -2.152000
 0.612000 2.099000 -1.121000
 -1.122000 -0.207000 -0.563000
 2.046000 2.011000 1.488000
 1.381000 0.208000 3.111000
 1.874000 -1.000000 1.928000
 3.088000 1.276000 -0.679000
 2.834000 -0.400000 -0.202000
 1.357000 -1.171000 -1.963000
 0.174000 -0.065000 -2.696000
 1.919000 0.308000 -2.771000
 -0.414000 2.113000 -1.504000
 0.667000 2.723000 -0.224000
 1.277000 2.539000 -1.874000
 -0.240000 2.156000 1.791000
 -1.758000 1.272000 1.480000
 -0.946000 1.148000 3.062000
 -1.762000 -1.276000 1.603000
 -0.220000 -2.157000 1.537000
 -0.696000 -1.328000 3.034000
 3.814000 0.868000 1.962000
 4.338000 -0.267000 1.879000
 4.270000 1.918000 2.463000
```

-1.184000 -0.083000 -0.992000
-1.456000 -0.403000 -0.335000
!entry.CTM.unit.residueconnect table int c1x int c2x int c3x int c4x int c5x int c6x
0 0 0 0 0 0
!entry.CTM.unit.residues table str name int seq int childseq int startatomx str restype int imagingx
"CTM" 1 34 1 "?" 0
!entry.CTM.unit.residuesPdbSequenceNumber array int
1
!entry.CTM.unit.solventcap array dbl
-1.000000
0.0
0.0
0.0
0.0
!entry.CTM.unit.velocities table dbl x dbl y dbl z
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
!entry.DMN.unit.atoms table str name str type int typex int resx int flags int seq int elmnt dbl chg
"N1" "NN" 0 1 131074 1 7 0.110000
"O2" "ON" 0 1 131074 2 8 -0.110000
"C3" "CT" 0 1 131074 3 6 -0.115000
"C4" "CT" 0 1 131074 4 6 -0.115000
"H5" "H1" 0 1 131074 5 1 0.075000
"H6" "H1" 0 1 131074 6 1 0.075000
"H7" "H1" 0 1 131074 7 1 0.075000
"H8" "H1" 0 1 131074 8 1 0.075000
"H9" "H1" 0 1 131074 9 1 0.075000
"H10" "H1" 0 1 131074 10 1 0.075000
"Lp1" "LP" 0 1 131074 11 0 -0.110000

```
 "Lp2" "LP" 0 1 131074 12 0 -0.110000
!entry.DMN.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "O2" "ON" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "H5" "H1" 0 -1 0.0
 "H6" "H1" 0 -1 0.0
 "H7" "H1" 0 -1 0.0
 "H8" "H1" 0 -1 0.0
 "H9" "H1" 0 -1 0.0
 "H10" "H1" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.DMN.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.DMN.unit.childsequence single int
 2
!entry.DMN.unit.connect array int
 0
 0
!entry.DMN.unit.connectivity table  int atom1x  int atom2x  int flags
 1 4 1
 1 3 1
 1 2 1
 2 11 1
 2 12 1
 3 8 1
 3 9 1
 3 10 1
 4 5 1
 4 7 1
 4 6 1
!entry.DMN.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
!entry.DMN.unit.name single str
 "DMNO"
!entry.DMN.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.268000
 1.277000 0.0 -0.686000
 -1.161000 0.531000 -0.686000
 -1.231000 0.105000 -1.692000
 -2.044000 0.262000 -0.104000
 -1.102000 1.628000 -0.765000
 1.163000 -0.416000 -1.692000
```

```
 1.680000 1.021000 -0.765000
 1.968000 -0.612000 -0.104000
 0.390000 0.0 1.493000
 -0.390000 0.0 1.493000
!entry.DMN.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.DMN.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "DMN" 1 13 1 "?" 0
!entry.DMN.unit.residuesPdbSequenceNumber array int
 1
!entry.DMN.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.DMN.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.DTB.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 -0.022000
 "O2" "ON" 0 1 131074 2 8 -0.060000
 "C3" "CT" 0 1 131074 3 6 0.187000
 "C4" "CT" 0 1 131074 4 6 0.187000
 "C5" "CT" 0 1 131074 5 6 -0.114000
 "H6" "HN" 0 1 131074 6 1 0.034000
 "H7" "HN" 0 1 131074 7 1 0.034000
 "H8" "HN" 0 1 131074 8 1 0.034000
 "C9" "CT" 0 1 131074 9 6 -0.114000
 "H10" "HN" 0 1 131074 10 1 0.034000
 "H11" "HN" 0 1 131074 11 1 0.034000
 "H12" "HN" 0 1 131074 12 1 0.034000
 "C13" "CT" 0 1 131074 13 6 -0.114000
 "H14" "HN" 0 1 131074 14 1 0.034000
 "H15" "HN" 0 1 131074 15 1 0.034000
 "H16" "HN" 0 1 131074 16 1 0.034000
 "C17" "CT" 0 1 131074 17 6 -0.114000
 "H18" "HN" 0 1 131074 18 1 0.034000
 "H19" "HN" 0 1 131074 19 1 0.034000
 "H20" "HN" 0 1 131074 20 1 0.034000
 "C21" "CT" 0 1 131074 21 6 -0.114000
 "H22" "HN" 0 1 131074 22 1 0.034000
 "H23" "HN" 0 1 131074 23 1 0.034000
 "H24" "HN" 0 1 131074 24 1 0.034000
 "C25" "CT" 0 1 131074 25 6 -0.114000
 "H26" "HN" 0 1 131074 26 1 0.034000
 "H27" "HN" 0 1 131074 27 1 0.034000
 "H28" "HN" 0 1 131074 28 1 0.034000
 "Lp1" "LP" 0 1 131074 29 0 -0.110000
 "Lp2" "LP" 0 1 131074 30 0 -0.110000
```

```
!entry.DTB.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "O2" "ON" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "H6" "HN" 0 -1 0.0
 "H7" "HN" 0 -1 0.0
 "H8" "HN" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "H10" "HN" 0 -1 0.0
 "H11" "HN" 0 -1 0.0
 "H12" "HN" 0 -1 0.0
 "C13" "CT" 0 -1 0.0
 "H14" "HN" 0 -1 0.0
 "H15" "HN" 0 -1 0.0
 "H16" "HN" 0 -1 0.0
 "C17" "CT" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "C21" "CT" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
 "C25" "CT" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "H27" "HN" 0 -1 0.0
 "H28" "HN" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.DTB.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.DTB.unit.childsequence single int
 2
!entry.DTB.unit.connect array int
 0
 0
!entry.DTB.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 1
 1 3 1
 1 4 1
 2 30 1
 2 29 1
 3 25 1
 3 21 1
 3 17 1
 4 9 1
 4 13 1
 4 5 1
 5 6 1
 5 7 1
 5 8 1
 9 12 1
 9 11 1
 9 10 1
 13 15 1
 13 14 1
```

```
 13 16 1
 17 20 1
 17 18 1
 17 19 1
 21 23 1
 21 24 1
 21 22 1
 25 27 1
 25 28 1
 25 26 1
!entry.DTB.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
!entry.DTB.unit.name single str
 "DTBN"
!entry.DTB.unit.positions table  dbl x  dbl y  dbl z
 0.003000 -0.482000 -0.186000
 -0.035000 -1.755000 -0.092000
 1.352000 0.157000 -0.013000
 -1.342000 0.163000 -0.012000
 -1.821000 -0.099000 1.423000
 -2.862000 0.222000 1.532000
 -1.759000 -1.168000 1.644000
 -1.220000 0.448000 2.156000
 -2.284000 -0.534000 -1.000000
 -2.322000 -1.607000 -0.806000
 -3.291000 -0.116000 -0.901000
 -1.945000 -0.380000 -2.030000
 -1.369000 1.661000 -0.306000
 -2.395000 2.009000 -0.152000
 -1.100000 1.880000 -1.342000
 -0.731000 2.246000 0.361000
 1.500000 0.743000 1.398000
 0.814000 1.573000 1.584000
```

```
 1.327000 -0.029000 2.153000
 2.519000 1.124000 1.527000
 2.397000 -0.946000 -0.195000
 2.290000 -1.730000 0.555000
 2.311000 -1.412000 -1.180000
 3.390000 -0.496000 -0.104000
 1.607000 1.226000 -1.084000
 1.041000 2.144000 -0.926000
 1.374000 0.836000 -2.079000
 2.669000 1.493000 -1.068000
 0.348000 -1.990000 -0.074000
 -0.432000 -1.967000 -0.075000
!entry.DTB.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.DTB.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "DTB" 1 31 1 "?" 0
!entry.DTB.unit.residuesPdbSequenceNumber array int
 1
!entry.DTB.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.DTB.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.IND.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "C1" "CF" 0 1 131074 1 6 0.069100
 "C2" "CE" 0 1 131074 2 6 -0.002200
 "C3" "CA" 0 1 131072 3 6 -0.147100
 "C4" "CA" 0 1 131072 4 6 -0.119700
```

```
 "C5" "CA" 0 1 131072 5 6 -0.154500
 "C6" "CA" 0 1 131072 6 6 -0.101600
 "C7" "CI" 0 1 131072 7 6 0.150700
 "C8" "C" 0 1 131072 8 6 0.400900
 "H1" "HA" 0 1 131072 9 1 0.151900
 "H2" "HA" 0 1 131072 10 1 0.137300
 "H3" "HA" 0 1 131072 11 1 0.145900
 "H4" "HA" 0 1 131072 12 1 0.142100
 "O1" "O" 0 1 131072 13 8 -0.467400
 "O2" "ON" 0 1 131072 14 8 -0.127800
 "N1" "NN" 0 1 131072 15 7 0.091200
 "C9" "CA" 0 1 131072 16 6 -0.015600
 "C10" "CA" 0 1 131072 17 6 -0.131600
 "C11" "CA" 0 1 131072 18 6 -0.131600
 "C12" "CA" 0 1 131072 19 6 -0.156700
 "H5" "HA" 0 1 131072 20 1 0.148700
 "C13" "CA" 0 1 131072 21 6 -0.156700
 "H6" "HA" 0 1 131072 22 1 0.148700
 "C14" "CA" 0 1 131072 23 6 -0.123900
 "H7" "HA" 0 1 131072 24 1 0.140200
 "H8" "HA" 0 1 131072 25 1 0.140200
 "H9" "HA" 0 1 131072 26 1 0.136500
 "C15" "CT" 0 1 131072 27 6 -0.081800
 "H10" "HC" 0 1 131072 28 1 0.044800
 "H11" "HC" 0 1 131072 29 1 0.044800
 "H12" "HC" 0 1 131072 30 1 0.044800
 "Lp1" "LP" 0 1 131072 31 0 -0.109800
 "Lp2" "LP" 0 1 131072 32 0 -0.109800
!entry.IND.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "C1" "CN" 0 -1 0.0
 "C2" "CB" 0 -1 0.0
 "C3" "CA" 0 -1 0.0
 "C4" "CA" 0 -1 0.0
 "C5" "CA" 0 -1 0.0
 "C6" "CA" 0 -1 0.0
 "C7" "CI" 0 -1 0.0
 "C8" "C" 0 -1 0.0
 "H1" "HA" 0 -1 0.0
 "H2" "HA" 0 -1 0.0
 "H3" "HA" 0 -1 0.0
 "H4" "HA" 0 -1 0.0
 "O1" "O" 0 -1 0.0
 "O2" "ON" 0 -1 0.0
 "N1" "NN" 0 -1 0.0
 "C9" "CA" 0 -1 0.0
 "C10" "CA" 0 -1 0.0
 "C11" "CA" 0 -1 0.0
 "C12" "CA" 0 -1 0.0
 "H5" "HA" 0 -1 0.0
 "C13" "CA" 0 -1 0.0
 "H6" "HA" 0 -1 0.0
 "C14" "CA" 0 -1 0.0
 "H7" "HA" 0 -1 0.0
 "H8" "HA" 0 -1 0.0
 "H9" "HA" 0 -1 0.0
 "C15" "CT" 0 -1 0.0
 "H10" "HC" 0 -1 0.0
 "H11" "HC" 0 -1 0.0
 "H12" "HC" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.IND.unit.boundbox array dbl
```

```
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.IND.unit.childsequence single int
 2
!entry.IND.unit.connect array int
 0
 0
!entry.IND.unit.connectivity table  int atom1x  int atom2x  int flags
 1 6 1
 1 2 1
 1 15 1
 2 3 1
 2 8 1
 3 4 1
 3 9 1
 4 5 1
 4 10 1
 5 6 1
 5 11 1
 6 12 1
 7 8 1
 7 15 1
 7 27 1
 7 16 1
 8 13 1
 14 15 1
 14 32 1
 14 31 1
 16 17 1
 16 18 1
 17 19 1
 17 20 1
 18 21 1
 18 22 1
 19 23 1
 19 24 1
 21 23 1
 21 25 1
 23 26 1
 27 30 1
 27 28 1
 27 29 1
!entry.IND.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
```

```
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
!entry.IND.unit.name single str
 "INDCO"
!entry.IND.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.402000
 1.199000 0.0 2.109000
 2.388000 0.007000 1.386000
 2.371000 0.001000 -0.020000
 1.183000 -0.006000 -0.741000
 -2.295000 0.037000 0.608000
 -1.392000 -0.047000 1.866000
 1.189000 -0.006000 3.196000
 3.341000 0.012000 1.908000
 3.316000 0.001000 -0.559000
 1.157000 -0.017000 -1.826000
 -1.800000 -0.156000 2.998000
 -1.604000 -0.120000 -1.700000
 -1.296000 -0.015000 -0.486000
 -3.054000 1.361000 0.607000
 -3.931000 1.634000 1.663000
 -2.904000 2.305000 -0.412000
 -4.646000 2.827000 1.696000
 -4.034000 0.920000 2.476000
 -3.624000 3.498000 -0.375000
 -2.242000 2.107000 -1.249000
 -4.497000 3.764000 0.676000
 -5.320000 3.025000 2.527000
 -3.500000 4.221000 -1.178000
 -5.057000 4.696000 0.701000
 -3.223000 -1.170000 0.511000
 -3.908000 -1.170000 1.362000
 -3.795000 -1.116000 -0.419000
 -2.649000 -2.103000 0.524000
 -1.281000 -0.157000 -2.011000
 -2.037000 -0.121000 -1.823000
!entry.IND.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.IND.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "IND" 1 33 1 "?" 0
!entry.IND.unit.residuesPdbSequenceNumber array int
 1
!entry.IND.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
```

```
 0.0
 0.0
!entry.IND.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.NIT.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "C1" "CT" 0 1 131072 1 6 -0.040000
 "C2" "CT" 0 1 131072 2 6 -0.040000
 "C3" "CX" 0 1 131072 3 6 0.260000
 "H1" "H1" 0 1 131072 4 1 0.096000
 "H2" "H1" 0 1 131072 5 1 0.096000
 "H3" "H1" 0 1 131072 6 1 0.096000
 "H4" "H1" 0 1 131072 7 1 0.096000
 "N1" "NN" 0 1 131072 8 7 0.145000
 "N2" "NN" 0 1 131072 9 7 0.145000
 "O1" "ON" 0 1 131072 10 8 -0.230000
 "O2" "ON" 0 1 131072 11 8 -0.230000
 "C4" "CT" 0 1 131072 12 6 -0.242000
 "H5" "HC" 0 1 131072 13 1 0.096000
 "H6" "HC" 0 1 131072 14 1 0.096000
 "H7" "HC" 0 1 131072 15 1 0.096000
 "Lp1" "LP" 0 1 131072 16 0 -0.110000
 "Lp2" "LP" 0 1 131072 17 0 -0.110000
 "Lp3" "LP" 0 1 131072 18 0 -0.110000
 "Lp4" "LP" 0 1 131072 19 0 -0.110000
!entry.NIT.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "C1" "CT" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CX" 0 -1 0.0
 "H1" "H1" 0 -1 0.0
 "H2" "H1" 0 -1 0.0
```

```
 "H3" "H1" 0 -1 0.0
 "H4" "H1" 0 -1 0.0
 "N1" "NN" 0 -1 0.0
 "N2" "NN" 0 -1 0.0
 "O1" "ON" 0 -1 0.0
 "O2" "ON" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "H5" "HC" 0 -1 0.0
 "H6" "HC" 0 -1 0.0
 "H7" "HC" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
 "Lp3" "LP" 0 -1 0.0
 "Lp4" "LP" 0 -1 0.0
!entry.NIT.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.NIT.unit.childsequence single int
 2
!entry.NIT.unit.connect array int
 0
 0
!entry.NIT.unit.connectivity table  int atom1x  int atom2x  int flags
 1 5 1
 1 4 1
 1 8 1
 1 2 1
 2 7 1
 2 6 1
 2 9 1
 3 9 1
 3 8 1
 3 12 1
 8 10 1
 9 11 1
 10 17 1
 10 16 1
 11 19 1
 11 18 1
 12 15 1
 12 13 1
 12 14 1
!entry.NIT.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
```

```
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
!entry.NIT.unit.name single str
 "NITNO"
!entry.NIT.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.529000
 2.201000 0.0 0.767000
 -0.454000 -0.890000 -0.444000
 -0.455000 0.890000 -0.444000
 -0.454000 -0.890000 1.973000
 -0.455000 0.890000 1.973000
 1.435000 0.0 -0.338000
 1.435000 0.001000 1.872000
 1.841000 0.0 -1.530000
 1.826000 0.002000 3.069000
 3.673000 -0.003000 0.758000
 4.052000 -0.600000 1.593000
 4.048000 -0.457000 -0.166000
 4.029000 1.027000 0.834000
 2.282000 0.0 -1.618000
 1.544000 0.0 -1.869000
 2.266000 0.002000 3.161000
 1.526000 0.001000 3.404000
!entry.NIT.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.NIT.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "NIT" 1 21 1 "?" 0
!entry.NIT.unit.residuesPdbSequenceNumber array int
 1
!entry.NIT.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.NIT.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.OPR.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "C1" "CT" 0 1 131072 1 6 -0.136000
 "C2" "CT" 0 1 131072 2 6 0.287000
```

```
 "C3" "CP" 0 1 131072 3 6 0.287000
 "H1" "HC" 0 1 131072 4 1 0.060000
 "H3" "HC" 0 1 131072 5 1 0.060000
 "N1" "NN" 0 1 131072 6 7 0.080000
 "O1" "ON" 0 1 131072 7 8 -0.184000
 "C4" "CT" 0 1 131072 8 6 -0.106000
 "H4" "HN" 0 1 131072 9 1 0.022000
 "H5" "HN" 0 1 131072 10 1 0.022000
 "H6" "HN" 0 1 131072 11 1 0.022000
 "C5" "CT" 0 1 131072 12 6 -0.106000
 "H7" "HN" 0 1 131072 13 1 0.022000
 "H8" "HN" 0 1 131072 14 1 0.022000
 "H9" "HN" 0 1 131072 15 1 0.022000
 "C6" "CT" 0 1 131072 16 6 -0.106000
 "H10" "HN" 0 1 131072 17 1 0.022000
 "H11" "HN" 0 1 131072 18 1 0.022000
 "H12" "HN" 0 1 131072 19 1 0.022000
 "C7" "CT" 0 1 131072 20 6 -0.106000
 "H13" "HN" 0 1 131072 21 1 0.022000
 "H14" "HN" 0 1 131072 22 1 0.022000
 "H15" "HN" 0 1 131072 23 1 0.022000
 "C8" "C" 0 1 131072 24 6 0.444000
 "O2" "O" 0 1 131072 25 8 -0.518000
 "Lp1" "LP" 0 1 131072 26 0 -0.110000
 "Lp2" "LP" 0 1 131072 27 0 -0.110000
!entry.OPR.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "C1" "CT" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CP" 0 -1 0.0
 "H1" "HC" 0 -1 0.0
 "H3" "HC" 0 -1 0.0
 "N1" "NN" 0 -1 0.0
 "O1" "ON" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "H4" "HN" 0 -1 0.0
 "H5" "HN" 0 -1 0.0
 "H6" "HN" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "H7" "HN" 0 -1 0.0
 "H8" "HN" 0 -1 0.0
 "H9" "HN" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "H10" "HN" 0 -1 0.0
 "H11" "HN" 0 -1 0.0
 "H12" "HN" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "H13" "HN" 0 -1 0.0
 "H14" "HN" 0 -1 0.0
 "H15" "HN" 0 -1 0.0
 "C8" "C" 0 -1 0.0
 "O2" "O" 0 -1 0.0
 "LP1" "LP" 0 -1 0.0
 "LP2" "LP" 0 -1 0.0
!entry.OPR.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.OPR.unit.childsequence single int
 2
!entry.OPR.unit.connect array int
```

```
 0
 0
!entry.OPR.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 1
 1 24 1
 1 5 1
 1 4 1
 2 6 1
 2 16 1
 2 20 1
 3 6 1
 3 24 1
 3 8 1
 3 12 1
 6 7 1
 7 26 1
 7 27 1
 8 9 1
 8 11 1
 8 10 1
 12 14 1
 12 13 1
 12 15 1
 16 18 1
 16 17 1
 16 19 1
 20 23 1
 20 22 1
 20 21 1
 24 25 1
!entry.OPR.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
!entry.OPR.unit.name single str
 "3-Oxo-PROXYL"
!entry.OPR.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
```

```
 0.0 0.0 1.532000
 2.374000 0.0 0.740000
 -0.685000 -0.725000 -0.447000
 -0.264000 0.991000 -0.394000
 1.429000 0.270000 1.835000
 1.824000 0.446000 3.018000
 3.221000 1.242000 0.459000
 3.801000 1.488000 1.354000
 3.902000 1.044000 -0.374000
 2.595000 2.104000 0.205000
 3.258000 -1.207000 1.052000
 3.910000 -1.411000 0.198000
 3.866000 -0.989000 1.935000
 2.661000 -2.101000 1.255000
 -0.856000 1.101000 2.145000
 -1.913000 0.924000 1.920000
 -0.725000 1.119000 3.230000
 -0.573000 2.082000 1.748000
 -0.385000 -1.367000 2.104000
 -0.185000 -1.387000 3.180000
 -1.451000 -1.560000 1.940000
 0.183000 -2.176000 1.630000
 1.428000 -0.283000 -0.422000
 1.779000 -0.662000 -1.510000
 2.259000 0.528000 3.100000
 1.530000 0.428000 3.359000
!entry.OPR.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.OPR.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "OPR" 1 28 1 "?" 0
!entry.OPR.unit.residuesPdbSequenceNumber array int
 1
!entry.OPR.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.OPR.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```

```
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.OTM.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 0.037000
 "C2" "CT" 0 1 131074 2 6 0.189000
 "C3" "CT" 0 1 131074 3 6 -0.055000
 "C4" "CT" 0 1 131074 4 6 -0.055000
 "C5" "CT" 0 1 131074 5 6 0.189000
 "C6" "CT" 0 1 131074 6 6 -0.089000
 "C7" "CT" 0 1 131074 7 6 -0.089000
 "C8" "CT" 0 1 131074 8 6 -0.089000
 "C9" "CT" 0 1 131074 9 6 -0.089000
 "O10" "ON" 0 1 131074 10 8 -0.118000
 "H11" "HC" 0 1 131074 11 1 0.034000
 "H12" "HC" 0 1 131074 12 1 0.034000
 "H13" "HC" 0 1 131074 13 1 0.034000
 "H14" "HC" 0 1 131074 14 1 0.034000
 "H15" "HN" 0 1 131074 15 1 0.027000
 "H16" "HN" 0 1 131074 16 1 0.027000
 "H17" "HN" 0 1 131074 17 1 0.027000
 "H18" "HN" 0 1 131074 18 1 0.027000
 "H19" "HN" 0 1 131074 19 1 0.027000
 "H20" "HN" 0 1 131074 20 1 0.027000
 "H21" "HN" 0 1 131074 21 1 0.027000
 "H22" "HN" 0 1 131074 22 1 0.027000
 "H23" "HN" 0 1 131074 23 1 0.027000
 "H24" "HN" 0 1 131074 24 1 0.027000
 "H25" "HN" 0 1 131074 25 1 0.027000
 "H26" "HN" 0 1 131074 26 1 0.027000
 "C27" "C" 0 1 131074 27 6 0.420000
 "O28" "O" 0 1 131074 28 8 -0.491000
 "Lp1" "LP" 0 1 131074 29 0 -0.110000
 "Lp2" "LP" 0 1 131074 30 0 -0.110000
!entry.OTM.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "O10" "ON" 0 -1 0.0
 "H11" "HC" 0 -1 0.0
 "H12" "HC" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HN" 0 -1 0.0
 "H16" "HN" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
```

```
 "H25" "HN" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "C27" "C" 0 -1 0.0
 "O28" "O" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.OTM.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.OTM.unit.childsequence single int
 2
!entry.OTM.unit.connect array int
 0
 0
!entry.OTM.unit.connectivity table  int atom1x  int atom2x  int flags
 1 10 1
 1 2 1
 1 5 1
 2 7 1
 2 6 1
 2 3 1
 3 12 1
 3 11 1
 3 27 1
 4 5 1
 4 13 1
 4 14 1
 4 27 1
 5 9 1
 5 8 1
 6 22 1
 6 23 1
 6 21 1
 7 24 1
 7 25 1
 7 26 1
 8 16 1
 8 17 1
 8 15 1
 9 18 1
 9 19 1
 9 20 1
 10 29 1
 10 30 1
 27 28 1
!entry.OTM.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
```

```
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
!entry.OTM.unit.name single str
 "4-Oxo-TEMPO"
!entry.OTM.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 -1.011000
 -1.311000 0.003000 -0.313000
 -1.142000 -0.578000 1.095000
 1.142000 0.578000 1.095000
 1.311000 -0.003000 -0.313000
 -1.840000 1.443000 -0.264000
 -2.280000 -0.872000 -1.106000
 1.840000 -1.443000 -0.264000
 2.280000 0.872000 -1.106000
 0.0 0.0 -2.277000
 -2.066000 -0.460000 1.670000
 -0.958000 -1.660000 1.024000
 0.958000 1.660000 1.024000
 2.066000 0.460000 1.670000
 1.211000 -2.094000 0.353000
 1.873000 -1.854000 -1.277000
 2.853000 -1.460000 0.153000
 2.447000 0.463000 -2.102000
 1.888000 1.888000 -1.213000
 3.239000 0.922000 -0.574000
 -1.211000 2.094000 0.353000
 -1.873000 1.854000 -1.277000
 -2.853000 1.460000 0.153000
 -2.447000 -0.463000 -2.102000
 -1.888000 -1.888000 -1.213000
 -3.239000 -0.922000 -0.574000
 0.0 0.0 1.898000
 0.0 0.0 3.107000
 -0.389000 0.002000 -2.502000
 0.389000 -0.002000 -2.502000
!entry.OTM.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.OTM.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "OTM" 1 31 1 "?" 0
!entry.OTM.unit.residuesPdbSequenceNumber array int
 1
!entry.OTM.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
```

```
 0.0
!entry.OTM.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.PRX.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "C1" "CT" 0 1 131072 1 6 0.287000
 "N1" "NN" 0 1 131072 2 7 0.080000
 "C2" "CT" 0 1 131072 3 6 0.287000
 "C3" "CT" 0 1 131072 4 6 -0.055000
 "C4" "CT" 0 1 131072 5 6 -0.055000
 "O1" "ON" 0 1 131072 6 8 -0.184000
 "C5" "CT" 0 1 131072 7 6 -0.106000
 "C6" "CT" 0 1 131072 8 6 -0.106000
 "C7" "CT" 0 1 131072 9 6 -0.106000
 "C8" "CT" 0 1 131072 10 6 -0.106000
 "H1" "HN" 0 1 131072 11 1 0.022000
 "H2" "HN" 0 1 131072 12 1 0.022000
 "H3" "HN" 0 1 131072 13 1 0.022000
 "H4" "HN" 0 1 131072 14 1 0.022000
 "H5" "HN" 0 1 131072 15 1 0.022000
 "H6" "HN" 0 1 131072 16 1 0.022000
 "H7" "HN" 0 1 131072 17 1 0.022000
 "H8" "HN" 0 1 131072 18 1 0.022000
 "H9" "HN" 0 1 131072 19 1 0.022000
 "H10" "HN" 0 1 131072 20 1 0.022000
 "H11" "HN" 0 1 131072 21 1 0.022000
 "H12" "HN" 0 1 131072 22 1 0.022000
 "H13" "HC" 0 1 131072 23 1 0.005000
 "H14" "HC" 0 1 131072 24 1 0.005000
 "H15" "HC" 0 1 131072 25 1 0.005000
 "H16" "HC" 0 1 131072 26 1 0.005000
 "Lp1" "LP" 0 1 131072 27 0 -0.110000
 "Lp2" "LP" 0 1 131072 28 0 -0.110000
```

```
!entry.PRX.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "C1" "CT" 0 -1 0.0
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "O1" "ON" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "H1" "HN" 0 -1 0.0
 "H2" "HN" 0 -1 0.0
 "H3" "HN" 0 -1 0.0
 "H4" "HN" 0 -1 0.0
 "H5" "HN" 0 -1 0.0
 "H6" "HN" 0 -1 0.0
 "H7" "HN" 0 -1 0.0
 "H8" "HN" 0 -1 0.0
 "H9" "HN" 0 -1 0.0
 "H10" "HN" 0 -1 0.0
 "H11" "HN" 0 -1 0.0
 "H12" "HN" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HC" 0 -1 0.0
 "H16" "HC" 0 -1 0.0
 "LP1" "LP" 0 -1 0.0
 "LP2" "LP" 0 -1 0.0
!entry.PRX.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.PRX.unit.childsequence single int
 2
!entry.PRX.unit.connect array int
 0
 0
!entry.PRX.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 1
 1 5 1
 1 10 1
 1 9 1
 2 6 1
 2 3 1
 3 4 1
 3 8 1
 3 7 1
 4 24 1
 4 23 1
 4 5 1
 5 26 1
 5 25 1
 6 28 1
 6 27 1
 7 12 1
 7 13 1
 7 11 1
 8 15 1
 8 16 1
```

```
 8 14 1
 9 18 1
 9 17 1
 9 19 1
 10 22 1
 10 20 1
 10 21 1
!entry.PRX.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
!entry.PRX.unit.name single str
 "PROXYL"
!entry.PRX.unit.positions table  dbl x  dbl y  dbl z
 1.250000 0.013000 0.126000
 0.0 0.0 -0.666000
 -1.250000 -0.013000 0.126000
 -0.709000 -0.291000 1.534000
 0.709000 0.291000 1.534000
 0.0 0.0 -1.932000
 -1.921000 1.360000 0.016000
 -2.179000 -1.102000 -0.397000
 2.179000 1.102000 -0.397000
 1.921000 -1.360000 0.016000
 -2.879000 1.359000 0.547000
 -1.292000 2.148000 0.441000
 -2.105000 1.598000 -1.036000
 -3.095000 -1.135000 0.202000
 -2.446000 -0.903000 -1.439000
 -1.695000 -2.083000 -0.350000
 3.095000 1.135000 0.202000
 2.446000 0.903000 -1.439000
 1.695000 2.083000 -0.350000
 2.879000 -1.359000 0.547000
 1.292000 -2.148000 0.441000
 2.105000 -1.598000 -1.036000
 -1.344000 0.148000 2.309000
```

```
 -0.676000 -1.373000 1.710000
 0.676000 1.373000 1.710000
 1.344000 -0.148000 2.309000
 0.311000 0.003000 -2.183000
 -0.311000 -0.003000 -2.183000
!entry.PRX.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.PRX.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "PRX" 1 32 1 "?" 0
!entry.PRX.unit.residuesPdbSequenceNumber array int
 1
!entry.PRX.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.PRX.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.TMP.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 196608 1 7 0.037000
 "C2" "CT" 0 1 196608 2 6 0.189000
 "C3" "CT" 0 1 196608 3 6 -0.073000
 "C4" "CT" 0 1 196608 4 6 -0.063000
 "C5" "CT" 0 1 196608 5 6 -0.073000
 "C6" "CT" 0 1 196608 6 6 0.189000
 "C7" "CT" 0 1 196608 7 6 -0.089000
 "C8" "CT" 0 1 196608 8 6 -0.089000
 "C9" "CT" 0 1 196608 9 6 -0.089000
 "C10" "CT" 0 1 196608 10 6 -0.089000
 "O1" "ON" 0 1 196608 11 8 -0.118000
 "H1" "HC" 0 1 196608 12 1 0.034000
 "H2" "HC" 0 1 196608 13 1 0.034000
```

```
 "H3" "HC" 0 1 196608 14 1 0.024000
 "H4" "HC" 0 1 196608 15 1 0.024000
 "H5" "HC" 0 1 196608 16 1 0.024000
 "H6" "HC" 0 1 196608 17 1 0.024000
 "H7" "HN" 0 1 196608 18 1 0.027000
 "H8" "HN" 0 1 196608 19 1 0.027000
 "H9" "HN" 0 1 196608 20 1 0.027000
 "H10" "HN" 0 1 196608 21 1 0.027000
 "H11" "HN" 0 1 196608 22 1 0.027000
 "H12" "HN" 0 1 196608 23 1 0.027000
 "H13" "HN" 0 1 196608 24 1 0.027000
 "H14" "HN" 0 1 196608 25 1 0.027000
 "H15" "HN" 0 1 196608 26 1 0.027000
 "H16" "HN" 0 1 196608 27 1 0.027000
 "H17" "HN" 0 1 196608 28 1 0.027000
 "H18" "HN" 0 1 196608 29 1 0.027000
 "Lp1" "LP" 0 1 196608 30 0 -0.110000
 "Lp2" "LP" 0 1 196608 31 0 -0.110000
!entry.TMP.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "O1" "ON" 0 -1 0.0
 "H1" "HC" 0 -1 0.0
 "H2" "HC" 0 -1 0.0
 "H3" "HC" 0 -1 0.0
 "H4" "HC" 0 -1 0.0
 "H5" "HC" 0 -1 0.0
 "H6" "HC" 0 -1 0.0
 "H7" "HN" 0 -1 0.0
 "H8" "HN" 0 -1 0.0
 "H9" "HN" 0 -1 0.0
 "H10" "HN" 0 -1 0.0
 "H11" "HN" 0 -1 0.0
 "H12" "HN" 0 -1 0.0
 "H13" "HN" 0 -1 0.0
 "H14" "HN" 0 -1 0.0
 "H15" "HN" 0 -1 0.0
 "H16" "HN" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.TMP.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TMP.unit.childsequence single int
 2
!entry.TMP.unit.connect array int
 0
 0
!entry.TMP.unit.connectivity table  int atom1x  int atom2x  int flags
```

```
 1 11 1
 1 2 1
 1 6 1
 2 3 1
 2 7 1
 2 8 1
 3 14 1
 3 15 1
 3 4 1
 4 12 1
 4 13 1
 4 5 1
 5 16 1
 5 17 1
 5 6 1
 6 10 1
 6 9 1
 7 25 1
 7 24 1
 7 26 1
 8 29 1
 8 27 1
 8 28 1
 9 19 1
 9 18 1
 9 20 1
 10 22 1
 10 23 1
 10 21 1
 11 31 1
 11 30 1
!entry.TMP.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
```

```
 "R" 1 "A" 31
!entry.TMP.unit.name single str
 "TEMPO"
!entry.TMP.unit.positions table  dbl x  dbl y  dbl z
 0.694000 0.206000 0.0
 0.022000 0.025000 1.318000
 -1.434000 0.500000 1.238000
 -2.166000 0.006000 0.0
 -1.434000 0.500000 -1.238000
 0.022000 0.025000 -1.318000
 0.108000 -1.451000 1.733000
 0.780000 0.877000 2.336000
 0.780000 0.877000 -2.336000
 0.108000 -1.451000 -1.733000
 1.961000 0.067000 0.0
 -2.238000 -1.089000 0.0
 -3.196000 0.380000 0.0
 -1.944000 0.182000 2.155000
 -1.445000 1.599000 1.237000
 -1.944000 0.182000 -2.155000
 -1.445000 1.599000 -1.237000
 0.798000 1.926000 -2.025000
 1.811000 0.533000 -2.441000
 0.280000 0.810000 -3.308000
 1.145000 -1.793000 -1.662000
 -0.514000 -2.098000 -1.109000
 -0.224000 -1.563000 -2.771000
 -0.514000 -2.098000 1.109000
 1.145000 -1.793000 1.662000
 -0.224000 -1.563000 2.771000
 1.811000 0.533000 2.441000
 0.798000 1.926000 2.025000
 0.280000 0.810000 3.308000
 2.180000 0.043000 0.272000
 2.180000 0.043000 -0.272000
!entry.TMP.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.TMP.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "TMP" 1 32 1 "?" 0
!entry.TMP.unit.residuesPdbSequenceNumber array int
 1
!entry.TMP.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TMP.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```

```
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
!entry.TNN.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 0.037000
 "C2" "CT" 0 1 131074 2 6 0.160000
 "C3" "CT" 0 1 131074 3 6 -0.063000
 "C4" "CT" 0 1 131074 4 6 0.098000
 "C5" "CT" 0 1 131074 5 6 -0.063000
 "C6" "CT" 0 1 131074 6 6 0.160000
 "C7" "CT" 0 1 131074 7 6 -0.089000
 "C8" "CT" 0 1 131074 8 6 -0.089000
 "C9" "CT" 0 1 131074 9 6 -0.089000
 "C10" "CT" 0 1 131074 10 6 -0.089000
 "O11" "ON" 0 1 131074 11 8 -0.118000
 "H12" "HP" 0 1 131074 12 1 0.057000
 "H13" "HC" 0 1 131074 13 1 0.057000
 "H14" "HC" 0 1 131074 14 1 0.057000
 "H15" "HC" 0 1 131074 15 1 0.057000
 "H16" "HC" 0 1 131074 16 1 0.057000
 "H17" "HN" 0 1 131074 17 1 0.027000
 "H18" "HN" 0 1 131074 18 1 0.027000
 "H19" "HN" 0 1 131074 19 1 0.027000
 "H20" "HN" 0 1 131074 20 1 0.027000
 "H21" "HN" 0 1 131074 21 1 0.027000
 "H22" "HN" 0 1 131074 22 1 0.027000
 "H23" "HN" 0 1 131074 23 1 0.027000
 "H24" "HN" 0 1 131074 24 1 0.027000
 "H25" "HN" 0 1 131074 25 1 0.027000
 "H26" "HN" 0 1 131074 26 1 0.027000
 "H27" "HN" 0 1 131074 27 1 0.027000
 "H28" "HN" 0 1 131074 28 1 0.027000
 "N29" "NT" 0 1 131074 29 7 -1.010000
 "H30" "H" 0 1 131074 30 1 0.383000
 "H31" "H" 0 1 131074 31 1 0.383000
 "Lp1" "LP" 0 1 131074 32 0 -0.110000
 "Lp2" "LP" 0 1 131074 33 0 -0.110000
!entry.TNN.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
```

```
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "O11" "ON" 0 -1 0.0
 "H12" "HP" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HC" 0 -1 0.0
 "H16" "HC" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
 "H25" "HN" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "H27" "HN" 0 -1 0.0
 "H28" "HN" 0 -1 0.0
 "N29" "NT" 0 -1 0.0
 "H30" "H" 0 -1 0.0
 "H31" "H" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.TNN.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TNN.unit.childsequence single int
 2
!entry.TNN.unit.connect array int
 0
 0
!entry.TNN.unit.connectivity table  int atom1x  int atom2x  int flags
 1 6 1
 1 11 1
 1 2 1
 2 8 1
 2 7 1
 2 3 1
 3 4 1
 3 14 1
 3 13 1
 4 5 1
 4 12 1
 4 29 1
 5 6 1
 5 15 1
 5 16 1
 6 9 1
 6 10 1
 7 24 1
 7 23 1
 7 25 1
 8 27 1
 8 26 1
 8 28 1
 9 19 1
 9 18 1
 9 17 1
```

```
 10 22 1
 10 20 1
 10 21 1
 11 33 1
 11 32 1
 29 30 1
 29 31 1
!entry.TNN.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
 "R" 1 "A" 33
!entry.TNN.unit.name single str
 "TANINE"
!entry.TNN.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.490000
 1.437000 0.0 2.021000
 2.356000 0.992000 1.326000
 2.392000 0.636000 -0.152000
 1.024000 0.682000 -0.840000
 -0.794000 1.214000 1.993000
 -0.705000 -1.279000 1.942000
 1.101000 -0.077000 -2.165000
 0.571000 2.124000 -1.113000
 -1.120000 -0.214000 -0.555000
 1.944000 2.010000 1.443000
 1.397000 0.200000 3.100000
 1.878000 -0.998000 1.899000
 3.065000 1.311000 -0.697000
 2.816000 -0.373000 -0.237000
 1.354000 -1.128000 -1.994000
 0.145000 -0.034000 -2.691000
```

```
 1.877000 0.370000 -2.796000
 -0.448000 2.118000 -1.512000
 0.588000 2.745000 -0.213000
 1.233000 2.586000 -1.855000
 -0.289000 2.161000 1.781000
 -1.778000 1.232000 1.515000
 -0.935000 1.142000 3.077000
 -1.742000 -1.291000 1.601000
 -0.198000 -2.162000 1.538000
 -0.687000 -1.338000 3.036000
 3.699000 0.874000 1.881000
 4.335000 1.522000 1.428000
 3.700000 1.100000 2.871000
 -1.189000 -0.086000 -0.981000
 -1.449000 -0.419000 -0.326000
!entry.TNN.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.TNN.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "TNN" 1 34 1 "?" 0
!entry.TNN.unit.residuesPdbSequenceNumber array int
 1
!entry.TNN.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TNN.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```

```
!entry.TNO.unit.atoms table  str name  str type  int typex  int resx  int flags  int seq
int elmnt  dbl chg
 "N1" "NN" 0 1 131074 1 7 0.037000
 "C2" "CT" 0 1 131074 2 6 0.160000
 "C3" "CT" 0 1 131074 3 6 -0.063000
 "C4" "CT" 0 1 131074 4 6 0.098000
 "C5" "CT" 0 1 131074 5 6 -0.063000
 "C6" "CT" 0 1 131074 6 6 0.160000
 "C7" "CT" 0 1 131074 7 6 -0.089000
 "C8" "CT" 0 1 131074 8 6 -0.089000
 "C9" "CT" 0 1 131074 9 6 -0.089000
 "C10" "CT" 0 1 131074 10 6 -0.089000
 "O11" "ON" 0 1 131074 11 8 -0.118000
 "H12" "H1" 0 1 131074 12 1 0.057000
 "H13" "HC" 0 1 131074 13 1 0.057000
 "H14" "HC" 0 1 131074 14 1 0.057000
 "H15" "HC" 0 1 131074 15 1 0.057000
 "H16" "HC" 0 1 131074 16 1 0.057000
 "H17" "HN" 0 1 131074 17 1 0.027000
 "H18" "HN" 0 1 131074 18 1 0.027000
 "H19" "HN" 0 1 131074 19 1 0.027000
 "H20" "HN" 0 1 131074 20 1 0.027000
 "H21" "HN" 0 1 131074 21 1 0.027000
 "H22" "HN" 0 1 131074 22 1 0.027000
 "H23" "HN" 0 1 131074 23 1 0.027000
 "H24" "HN" 0 1 131074 24 1 0.027000
 "H25" "HN" 0 1 131074 25 1 0.027000
 "H26" "HN" 0 1 131074 26 1 0.027000
 "H27" "HN" 0 1 131074 27 1 0.027000
 "H28" "HN" 0 1 131074 28 1 0.027000
 "O29" "OH" 0 1 131074 29 8 -0.674000
 "H30" "HO" 0 1 131074 30 1 0.430000
 "Lp1" "LP" 0 1 131074 31 0 -0.110000
 "Lp2" "LP" 0 1 131074 32 0 -0.110000
!entry.TNO.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
 "N1" "NN" 0 -1 0.0
 "C2" "CT" 0 -1 0.0
 "C3" "CT" 0 -1 0.0
 "C4" "CT" 0 -1 0.0
 "C5" "CT" 0 -1 0.0
 "C6" "CT" 0 -1 0.0
 "C7" "CT" 0 -1 0.0
 "C8" "CT" 0 -1 0.0
 "C9" "CT" 0 -1 0.0
 "C10" "CT" 0 -1 0.0
 "O11" "ON" 0 -1 0.0
 "H12" "H1" 0 -1 0.0
 "H13" "HC" 0 -1 0.0
 "H14" "HC" 0 -1 0.0
 "H15" "HC" 0 -1 0.0
 "H16" "HC" 0 -1 0.0
 "H17" "HN" 0 -1 0.0
 "H18" "HN" 0 -1 0.0
 "H19" "HN" 0 -1 0.0
 "H20" "HN" 0 -1 0.0
 "H21" "HN" 0 -1 0.0
 "H22" "HN" 0 -1 0.0
 "H23" "HN" 0 -1 0.0
 "H24" "HN" 0 -1 0.0
 "H25" "HN" 0 -1 0.0
 "H26" "HN" 0 -1 0.0
 "H27" "HN" 0 -1 0.0
```

```
 "H28" "HN" 0 -1 0.0
 "O29" "OH" 0 -1 0.0
 "H30" "HO" 0 -1 0.0
 "Lp1" "LP" 0 -1 0.0
 "Lp2" "LP" 0 -1 0.0
!entry.TNO.unit.boundbox array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TNO.unit.childsequence single int
 2
!entry.TNO.unit.connect array int
 0
 0
!entry.TNO.unit.connectivity table  int atom1x  int atom2x  int flags
 1 6 1
 1 11 1
 1 2 1
 2 8 1
 2 7 1
 2 3 1
 3 4 1
 3 14 1
 3 13 1
 4 5 1
 4 12 1
 4 29 1
 5 6 1
 5 15 1
 5 16 1
 6 9 1
 6 10 1
 7 24 1
 7 23 1
 7 25 1
 8 27 1
 8 26 1
 8 28 1
 9 19 1
 9 18 1
 9 17 1
 10 22 1
 10 20 1
 10 21 1
 11 31 1
 11 32 1
 29 30 1
!entry.TNO.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
 "U" 0 "R" 1
 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
 "R" 1 "A" 8
 "R" 1 "A" 9
 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
```

```
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
 "R" 1 "A" 16
 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
!entry.TNO.unit.name single str
 "TANOL"
!entry.TNO.unit.positions table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 1.490000
 1.437000 0.0 2.023000
 2.358000 0.983000 1.324000
 2.389000 0.652000 -0.157000
 1.017000 0.696000 -0.838000
 -0.790000 1.217000 1.995000
 -0.707000 -1.277000 1.943000
 1.090000 -0.048000 -2.172000
 0.559000 2.139000 -1.093000
 -1.119000 -0.220000 -0.555000
 1.999000 2.012000 1.474000
 1.410000 0.208000 3.100000
 1.875000 -1.000000 1.903000
 3.063000 1.338000 -0.684000
 2.818000 -0.354000 -0.257000
 1.344000 -1.101000 -2.013000
 0.133000 0.001000 -2.695000
 1.865000 0.407000 -2.799000
 -0.465000 2.136000 -1.479000
 0.584000 2.754000 -0.188000
 1.211000 2.609000 -1.837000
 -0.280000 2.163000 1.790000
 -1.771000 1.242000 1.512000
 -0.936000 1.140000 3.078000
 -1.746000 -1.284000 1.607000
 -0.206000 -2.161000 1.536000
 -0.685000 -1.337000 3.037000
 3.671000 0.855000 1.859000
 3.945000 1.695000 2.230000
 -1.189000 -0.089000 -0.980000
 -1.446000 -0.428000 -0.326000
!entry.TNO.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 0 0 0 0 0 0
!entry.TNO.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
 "TNO" 1 34 1 "?" 0
!entry.TNO.unit.residuesPdbSequenceNumber array int
 1
```

```
!entry.TNO.unit.solventcap array dbl
 -1.000000
 0.0
 0.0
 0.0
 0.0
!entry.TNO.unit.velocities table  dbl x  dbl y  dbl z
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
 0.0 0.0 0.0
```