```
==============================================================================================================================
PLATON(V-280799)-Run for: Nardelli  (Sucrose)                                                         TIME: Aug 17 11:20:51 1999
==============================================================================================================================
                                                                                                          (C) 1980-99 A.L.Spek
                                                       ============
====================================================== Crystal Data =========================================================
                                                       ============
                        Input Cell  (Lattice Type: P)                                    Reduced Cell (Acta Cryst. (1976),A32,297)
---------------------------------------------------------------------------------   ------------------------------------------------
a =    10.8633(5)  Angstrom                alpha =           90 Degree              a  =    7.758     alpha  =   90.00  V  =   715.0
b =     8.7050(4)                           beta =    102.945(6)                    b  =    8.705     beta   =  102.95
c =     7.7585(4)                          gamma =           90                     c  =   10.863     gamma  =   90.00

V =     715.04(6)  Cubic-Angstrom   Lambda(??Ka) =            0 Angstrom                         Niggli Values
                                                                                           60.190    75.780   118.010
                                                                                            0.000   -18.880     0.000
                                                ==========================
=============================================== Orthogonalization Matrices ===================================================
                                                ==========================

(See e.g. J.D.Dunitz, Xray Analysis and Structure determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(XO)   (  10.86330         0  -1.73803 ) (X)   ,   (X)   (   0.09205         0   0.02116 ) (XO)      Orthogonal Axes AO, BO and CO
(YO) = (         0   8.70500         0 )*(Y)   ,   (Y) = (         0   0.11488         0 )*(YO)            are defined as:
(ZO)   (         0         0   7.56132 ) (Z)   ,   (Z)   (         0         0   0.13225 ) (ZO)     AO // A, CO // C*, BO // CO X AO

                                                  ====================
================================================= Space Group Symmetry =======================================================
                                                  ====================

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21                   No:   4, Laue:  2/m [Hall:  P 2yb           ]

Lattice Type mP, Acentric,   Monoclinic, Order   2( 2) [Schoenflies: C2^2      ]

CHIRAL  - See P.G. Jones, Acta Cryst. (1986), A42, 57.

  Nr            ***** Symmetry Operation(s) *****

   1               X ,               Y ,               Z
   2             - X ,        1/2 + Y ,             - Z
```

```
=====================================================================================================================================
ADDSYM - CHECK  (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)
-------------------------------------------------------------------------------------------------------------------------------------

- This ADDSYM Search is run on ALL NON-H Chemical Types
- Number of Input Atoms Included in Search  =    23
- Density based on Input Atom set = 1.590 g.cm-3 - Vol / Non-H atom = 15.5 Ang^3
- The Structure implies the following Symmetry Elements subject to the Criteria:
   1.00 Deg., (metric)  0.25 Ang. (distances) and   0.45 Ang. (inv. and transl.)
- Percentage allowed NonFits =   20%

Symm.  Input  Reduced  (Ang)        (Deg) (%)   (Ang)                Input Cell
Elem Cell_Row Cell_Row   d  Typ Dot Angle Fit  MaxDev.            x     y     z
--------------------------------------------------------------------------------
 2   [ 0 1 0] [ 0-1 0]  8.71  2  1  0.00  100       0  through   1/2     0   1/2
  1                                                    Screw =     0   1/2     0

         T.R.A.N.S.F.O.R.M.A.T.I.O.N  M.A.T.R.I.X for CELL and HKL DATA
         ==============================================================
   Reduced->Convent         Input->Reduced       T = Input->Convent:    a' = T a
--------------------------------------------------------------------------------
(    -1     0     0 )   (     0     0     1 )   (     0     0    -1 )     Det(T)
(     0     1     0 ) X (     0    -1     0 ) = (     0    -1     0 )       =
(     0     0    -1 )   (     1     0     0 )   (    -1     0     0 )     1.000

Cell Lattice  a       b       c    alpha   beta  gamma Volume CrystalSystem Laue
--------------------------------------------------------------------------------
Input   mP 10.863   8.705   7.759  90.00 102.94  90.00    715   Monoclinic   2/m
Reduced  P  7.758   8.705  10.863  90.00 102.95  90.00    715
Convent mP  7.759   8.705  10.863  90.00 102.94  90.00    715   Monoclinic   2/m

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

::   * Caveat: Only a Limited Check for Missed Sub/Superlattice done. *
```

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

```
          Site    = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
*******   Move    = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
SYMBOLS:  Type    = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
*******   El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
          ARU     = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
          RESIDUE = collection of ARU’s constituting an isolated unit (= molecule, ion).
```

Atom Types :	C	H	O
Cov.Rad(Ang):	0.68	0.23	0.68
Atom Number :	6	1	8
Atom Weight :	12.010	1.008	16.00
Scat.Fact.f0:	5.999	1.000	7.999

Atom	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site SSN	*SSOF =	S.O.F	Move	Type
1	O(1)	0.17143(9)	0.34630(15)	0.39165(13)	1.182(1)	3.015(1)	2.961(1)	1	1	1	-	D/A
2	O(2)	0.22954(12)	0.43550(19)	0.74766(16)	1.194(1)	3.791(2)	5.653(1)	1	1	1	-	D/A
3	O(3)	0.30801(13)	0.74770(19)	0.7028(2)	2.125(1)	6.509(2)	5.314(2)	1	1	1	-	D/A
4	O(4)	0.34880(18)	0.8141(2)	0.3563(2)	3.170(2)	7.087(2)	2.694(2)	1	1	1	-	D/A
5	O(5)	0.37719(10)	0.39878(16)	0.36864(15)	3.457(1)	3.471(1)	2.787(1)	1	1	1	-	D/A
6	O(6)	0.58144(13)	0.5453(2)	0.2862(2)	5.819(1)	4.747(2)	2.164(2)	1	1	1	-	D/A
7	O(11)	0.03017(12)	0.2355(2)	0.62119(16)	-0.752(1)	2.050(2)	4.697(1)	1	1	1	-	D/A
8	O(21)	0.21205(10)	0.09445(16)	0.31572(13)	1.755(1)	0.822(1)	2.387(1)	1	1	1	-	D/A
9	O(31)	-0.07367(11)	0.31776(17)	0.20452(16)	-1.156(1)	2.766(1)	1.546(1)	1	1	1	-	D/A
10	O(41)	-0.02123(12)	0.09734(19)	-0.08904(14)	-0.076(1)	0.847(2)	-0.673(1)	1	1	1	-	D/A
11	O(61)	0.32644(13)	0.2380(2)	0.04035(17)	3.476(1)	2.072(2)	0.305(1)	1	1	1	-	D/A
12	C(1)	0.29961(8)	0.35792	0.48487(12)	2.412(1)	3.116(1)	3.666(1)	1	1	1	-	-
13	C(2)	0.31253(9)	0.47474(15)	0.63600(12)	2.290(1)	4.133(1)	4.809(1)	1	1	1	-	-
14	C(3)	0.28545(9)	0.63673(15)	0.56447(13)	2.120(1)	5.543(1)	4.268(1)	1	1	1	-	-
15	C(4)	0.37404(10)	0.67095(15)	0.44198(14)	3.295(1)	5.841(1)	3.342(1)	1	1	1	-	-
16	C(5)	0.35925(9)	0.55107(16)	0.29529(13)	3.389(1)	4.797(1)	2.233(1)	1	1	1	-	-
17	C(6)	0.45754(11)	0.57083(17)	0.18455(14)	4.650(1)	4.969(1)	1.395(1)	1	1	1	-	-
18	C(11)	0.10301(10)	0.13110(15)	0.54380(12)	0.174(1)	1.141(1)	4.112(1)	1	1	1	-	-
19	C(21)	0.12446(8)	0.19262(14)	0.36895(10)	0.711(1)	1.677(1)	2.790(1)	1	1	1	-	-
20	C(31)	0.00718(8)	0.19075(15)	0.21485(11)	-0.295(1)	1.660(1)	1.625(1)	1	1	1	-	-
21	C(41)	0.06478(9)	0.16653(15)	0.05476(11)	0.609(1)	1.450(1)	0.414(1)	1	1	1	-	-
22	C(51)	0.17635(9)	0.06133(15)	0.12864(12)	1.692(1)	0.534(1)	0.973(1)	1	1	1	-	-
23	C(61)	0.28927(10)	0.08194(17)	0.04668(14)	3.061(1)	0.713(1)	0.353(1)	1	1	1	-	-
24	H(1)	0.3347(2)	0.2451(3)	0.5388(3)	2.699(2)	2.134(3)	4.074(2)	1	1	1	-	-
25	H(2)	0.4116(2)	0.4693(3)	0.7117(3)	3.234(2)	4.085(3)	5.381(2)	1	1	1	-	-
26	H(3)	0.1871(2)	0.6448(3)	0.4897(3)	1.181(2)	5.613(3)	3.703(2)	1	1	1	-	-
27	H(4)	0.4717(2)	0.6681(3)	0.5218(3)	4.217(2)	5.816(3)	3.945(2)	1	1	1	-	-
28	H(5)	0.2638(2)	0.5613(3)	0.2093(3)	2.502(2)	4.886(3)	1.583(2)	1	1	1	-	-
29	H(6)	0.4531(3)	0.6873(4)	0.1345(4)	4.688(3)	5.983(3)	1.017(3)	1	1	1	-	-
30	H(11)	0.0520(3)	0.0224(3)	0.5216(4)	-0.342(3)	0.195(3)	3.944(3)	1	1	1	-	-
31	H(12)	0.1947(2)	0.1091(4)	0.6330(3)	1.015(2)	0.950(3)	4.786(2)	1	1	1	-	-

32	H(23)	0.2719(3)	0.3724(4)	0.8466(3)	1.482(3)	3.242(3)	6.401(2)	1	1	1	-	D-H
33	H(31)	-0.0495(2)	0.0884(3)	0.2290(3)	-0.936(2)	0.770(3)	1.732(2)	1	1	1	-	-
34	H(33)	0.2318(3)	0.7660(4)	0.7426(4)	1.227(3)	6.668(3)	5.615(3)	1	1	1	-	D-H
35	H(41)	0.0984(2)	0.2772(3)	0.0155(3)	1.042(2)	2.413(3)	0.117(2)	1	1	1	-	-
36	H(43)	0.3407(6)	0.8913(4)	0.4325(6)	2.949(7)	7.759(3)	3.270(5)	1	1	1	-	D-H
37	H(51)	0.1465(3)	-0.0599(3)	0.1133(3)	1.395(3)	-0.521(3)	0.857(2)	1	1	1	-	-
38	H(61)	0.4372(3)	0.4927(5)	0.0719(4)	4.624(3)	4.289(4)	0.544(3)	1	1	1	-	-

39	H(62)	0.2651(3)	0.0399(4)	-0.0887(4)	3.034(3)	0.347(3)	-0.671(3)	1	1	1	-	-
40	H(63)	0.6015(3)	0.4383(4)	0.2866(5)	6.036(3)	3.815(3)	2.167(4)	1	1	1	-	D-H
41	H(101)	0.0845(3)	0.3247(3)	0.6542(3)	-0.219(3)	2.827(3)	4.947(2)	1	1	1	-	D-H
42	H(301)	-0.0310(2)	0.4089(3)	0.1761(3)	-0.643(2)	3.559(3)	1.332(2)	1	1	1	-	D-H
43	H(401)	-0.0167(3)	0.1538(3)	-0.1961(3)	0.159(3)	1.339(3)	-1.483(2)	1	1	1	-	D-H
44	H(601)	0.3477(3)	0.2780(4)	0.1603(3)	3.499(3)	2.420(3)	1.212(2)	1	1	1	-	D-H
45	H(611)	0.3672(3)	0.0119(4)	0.1195(5)	3.781(3)	0.104(3)	0.904(4)	1	1	1	-	-

Ordered Structure   Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Res.Mol.Wt.	Z	C	H	O
1	1	0.233	0.366	0.345	342.30	2	12	22	11
Unit Cell Weight =					684.59		24	44	22
Calculated Analysis (Percent) =							42.1	6.5	51.4

Moiety_Formula = C12 H22 O11

Sum_Formula = C12 H22 O11

Formula_Weight = 342.30

Formula_Z = 2

SpaceGroup_Z = 2 ===> Z' = 2 / 2 = 1.000

Calculated Density = 1.5898(1) g cm-3 [= Mg m-3]

F(000) = 364.0 [363.97]

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

==

SYMMOL: Search for (additional) Molecular (Point Group) Symmetry - Hydrogen Atoms excluded !

==

For Details on the Molecular Symmetry Determination see: T. Pilati & A. Forni, J.Appl.Cryst. (1998), 31, 503-504

For CSM (i.e. Continuous Symmetry Measure), see: H. Zabrodsky et al. (1993) JACS, 115, 8278-8298

:: Resd # 1, No Molecular Symmetry Within Tolerance = 0.80 Ang.

NONSYM Search for Additional (Non)Crystallographic Symmetry between Residues (Experimental)

- Residue numbers with opposite signs indicate potential enantiomeric pairs
- Hydrogen atoms omitted from the analysis
- Residues with more than 6 atoms are analysed only

```
RES# Coords Center of Gravity        Main axes (hor)   EigenV   Asym Angle a,b,c
--------------------------------------------------------------------------------
 -1  0.2315   0.3668   0.3460   -0.549  0.632 -0.547    2852   37.76 123  51 114
     1.9137   3.1927   2.6160    0.684 -0.036 -0.729    2126   24.91  47  92 150
       Res.Mol.Wt. =   320.12    0.480  0.774  0.412    1305   50.85  61  39  73
```

(An)isotropic (Oblique/Cartesian), Equivalent and Main Axes Thermal Parameters - Unusual Values Marked with a #

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	O(1)	0.0154(4)	0.0131(4)	0.0177(4)	0.0006(3)	0.0035(3)	-0.0002(3)	0.0154(2)	0.0130	0.0154	0.0179	1.38
2	O(2)	0.0277(6)	0.0288(6)	0.0193(5)	-0.0013(4)	0.0084(4)	-0.0031(5)	0.0248(3)	0.0173	0.0253	0.0317	1.83
3	O(3)	0.0328(7)	0.0252(6)	0.0478(8)	-0.0172(6)	0.0206(6)	-0.0099(5)	0.0334(4)	0.0159	0.0232	0.0612	3.86
4	O(4)	0.0592(10)	0.0183(6)	0.0472(8)	0.0090(6)	0.0240(8)	0.0071(6)	0.0397(5)	0.0157	0.0369	0.0665	4.24
5	O(5)	0.0179(5)	0.0170(5)	0.0242(5)	-0.0006(4)	0.0091(4)	0.0000(4)	0.0190(3)	0.0143	0.0170	0.0257	1.79
6	O(6)	0.0218(5)	0.0337(7)	0.0413(7)	-0.0063(6)	0.0154(5)	-0.0055(5)	0.0310(4)	0.0159	0.0302	0.0468	2.95
7	O(11)	0.0286(5)	0.0330(6)	0.0200(5)	-0.0008(4)	0.0127(4)	-0.0035(5)	0.0261(3)	0.0137	0.0289	0.0356	2.60
8	O(21)	0.0227(5)	0.0181(5)	0.0156(4)	-0.0005(3)	0.0032(3)	0.0058(4)	0.0190(3)	0.0140	0.0156	0.0273	1.94
9	O(31)	0.0191(5)	0.0231(5)	0.0248(5)	0.0021(4)	0.0051(4)	0.0051(4)	0.0223(3)	0.0156	0.0241	0.0272	1.74
10	O(41)	0.0285(6)	0.0321(6)	0.0157(4)	-0.0020(4)	0.0016(4)	-0.0066(5)	0.0260(3)	0.0149	0.0255	0.0375	2.52
11	O(61)	0.0314(6)	0.0357(7)	0.0247(6)	0.0012(5)	0.0105(4)	-0.0058(6)	0.0299(4)	0.0201	0.0300	0.0397	1.98
12	C(1)	0.0156(3)	0.0144(3)	0.0169(3)	0.0001(3)	0.0038(3)	0.0003(3)	0.0156(2)	0.0143	0.0156	0.0169	1.18
13	C(2)	0.0173(3)	0.0191(4)	0.0186(4)	-0.0021(3)	0.0030(3)	-0.0020(3)	0.0185(2)	0.0152	0.0192	0.0210	1.38
14	C(3)	0.0182(4)	0.0168(4)	0.0280(4)	-0.0024(3)	0.0079(3)	-0.0008(3)	0.0206(2)	0.0163	0.0167	0.0287	1.76
15	C(4)	0.0227(4)	0.0155(4)	0.0291(4)	0.0002(4)	0.0099(4)	-0.0010(3)	0.0218(2)	0.0152	0.0198	0.0304	1.99
16	C(5)	0.0178(4)	0.0202(4)	0.0219(4)	0.0021(3)	0.0054(3)	-0.0010(3)	0.0198(2)	0.0164	0.0197	0.0233	1.43
17	C(6)	0.0298(5)	0.0288(5)	0.0249(4)	0.0000(4)	0.0125(4)	-0.0062(4)	0.0268(3)	0.0170	0.0271	0.0365	2.15
18	C(11)	0.0263(5)	0.0215(4)	0.0150(3)	0.0035(3)	0.0062(3)	-0.0033(4)	0.0207(2)	0.0120	0.0218	0.0282	2.35
19	C(21)	0.0174(3)	0.0139(3)	0.0123(3)	0.0011(3)	0.0041(2)	-0.0002(3)	0.0144(2)	0.0114	0.0144	0.0174	1.53
20	C(31)	0.0164(3)	0.0165(3)	0.0151(3)	0.0006(3)	0.0043(3)	-0.0014(3)	0.0159(2)	0.0138	0.0160	0.0179	1.30
21	C(41)	0.0201(3)	0.0182(4)	0.0134(3)	0.0000(3)	0.0043(3)	-0.0018(3)	0.0171(2)	0.0131	0.0171	0.0212	1.62
22	C(51)	0.0223(4)	0.0169(4)	0.0164(3)	-0.0020(3)	0.0062(3)	0.0013(3)	0.0182(2)	0.0134	0.0186	0.0227	1.69
23	C(61)	0.0274(5)	0.0305(5)	0.0236(4)	-0.0016(4)	0.0123(4)	0.0038(4)	0.0261(3)	0.0156	0.0295	0.0333	2.14
24	H(1)	0.0289(9)	0.0234(8)	0.0335(10)	0.0053(7)	0.0045(7)	0.0035(7)	0.0290(5)	0.0200	0.0306	0.0364	1.82
25	H(2)	0.0250(9)	0.0432(12)	0.0325(10)	-0.0028(9)	-0.0026(8)	-0.0009(9)	0.0350(6)	0.0204	0.0400	0.0445	2.18
26	H(3)	0.0234(9)	0.0364(12)	0.0507(13)	0.0015(10)	0.0059(9)	0.0028(8)	0.0372(7)	0.0228	0.0369	0.0519	2.28
27	H(4)	0.0285(10)	0.0429(13)	0.0423(11)	-0.0051(10)	0.0092(8)	-0.0085(9)	0.0377(7)	0.0245	0.0394	0.0492	2.01
28	H(5)	0.0279(9)	0.0436(13)	0.0390(11)	0.0050(10)	-0.0011(8)	0.0005(10)	0.0382(6)	0.0245	0.0405	0.0496	2.03
29	H(6)	0.0625(18)	0.0465(16)	0.0577(17)	0.0217(14)	0.0246(14)	-0.0005(14)	0.0538(10)	0.0253	0.0594	0.0768	3.03
30	H(11)	0.0641(17)	0.0307(12)	0.0413(12)	0.0027(10)	0.0177(12)	-0.0161(12)	0.0444(8)	0.0211	0.0416	0.0706	3.34
31	H(12)	0.0416(11)	0.0513(15)	0.0282(9)	0.0120(10)	0.0041(9)	0.0068(11)	0.0410(7)	0.0224	0.0434	0.0571	2.55
32	H(23)	0.0480(13)	0.0481(14)	0.0281(10)	0.0062(10)	0.0070(9)	-0.0035(12)	0.0416(7)	0.0261	0.0448	0.0540	2.07
33	H(31)	0.0316(10)	0.0279(10)	0.0323(9)	0.0008(8)	0.0086(8)	-0.0084(8)	0.0304(6)	0.0203	0.0324	0.0384	1.89
34	H(33)	0.0504(15)	0.0402(13)	0.0646(17)	-0.0199(13)	0.0337(14)	-0.0118(12)	0.0485(9)	0.0270	0.0329	0.0855	3.16
35	H(41)	0.0361(10)	0.0287(10)	0.0319(10)	0.0077(8)	0.0111(8)	-0.0027(8)	0.0317(6)	0.0199	0.0369	0.0382	1.92
36	H(43)	0.175(5)	0.0267(13)	0.083(3)	0.0050(16)	0.073(3)	0.017(2)	0.088(2)	0.0245	0.0528	0.1866	7.60
37	H(51)	0.0480(12)	0.0234(9)	0.0349(10)	-0.0051(8)	0.0109(9)	-0.0034(9)	0.0352(6)	0.0214	0.0356	0.0485	2.26
38	H(61)	0.0581(17)	0.074(2)	0.0368(12)	-0.0185(13)	0.0184(12)	-0.0206(16)	0.0551(10)	0.0286	0.0447	0.0919	3.21
39	H(62)	0.0633(16)	0.0557(17)	0.0355(11)	-0.0154(12)	0.0235(12)	-0.0054(15)	0.0495(9)	0.0220	0.0545	0.0721	3.27
40	H(63)	0.0505(16)	0.0404(15)	0.0614(18)	0.0083(13)	0.0138(13)	0.0012(13)	0.0506(9)	0.0375	0.0499	0.0643	1.72
41	H(101)	0.0490(14)	0.0347(12)	0.0431(12)	-0.0069(10)	0.0206(11)	-0.0064(11)	0.0406(7)	0.0305	0.0335	0.0579	1.90
42	H(301)	0.0407(12)	0.0260(10)	0.0460(12)	0.0053(9)	0.0133(10)	0.0040(9)	0.0370(7)	0.0244	0.0379	0.0487	2.00
43	H(401)	0.0482(13)	0.0426(13)	0.0211(9)	0.0016(8)	0.0018(9)	-0.0001(11)	0.0382(7)	0.0207	0.0427	0.0514	2.48
44	H(601)	0.0516(15)	0.0484(15)	0.0357(12)	-0.0066(11)	0.0116(11)	-0.0098(12)	0.0449(8)	0.0329	0.0417	0.0603	1.83

45	H(611)	0.0422(14)	0.0592(19)	0.0661(19)	0.0164(15)	0.0189(13)	0.0216(14)	0.0548(10)	0.0274	0.0522	0.0846	3.09

=====================

The Temperature Factor has the Form of Exp(-T)

where

T = 8*(pi**2)*Uiso*sin(theta/lambda)**2, for Isotropic Atoms,

T = 2*(pi**2)*(U11*(h*as)**2+U22*(k*bs)**2+U33*(l*cs)**2+2*U23*k*l*bs*cs+2*U13*h*l*as*cs+2*U12*h*k*as*bs),for Anisotr. Atoms

Ueq = 1/3 Sum(i,j) (Uij*as(i)*as(j)*a(i).a(j))

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	O
Average	0.0227	0.0196	0.0437	0.0261
Minimum	0.0144	0.0144	0.0290	0.0154
Maximum	0.0397	0.0268	0.0880	0.0397
Ratio	2.7569	1.8611	3.0345	2.5779
Number	23	12	22	11

Schomaker and Trueblood Rigid Body Motion Analysis, TLS - Model   (Acta Cryst. (1968), B24, 63) - see also Dunitz, p244

Vibration Tensor in Inertial System I(1)=L,I(2)=M, I(3)=N (Difference U(calc)-U(obs) in Parentheses)

Label	U(L,L)	U(L,M)	U(L,N)	U(M,M)	U(M,N)	U(N,N)	Ueq(obs)	Ueq(cal)
O(1)	0.01437(0.00488)	0.00109(-.00102)	-0.00149(-.00052)	0.01719(-.00284)	-0.00050(0.00071)	0.01474(-.00310)	0.0154	0.0151
O(2)	0.02527(-.00429)	-0.00100(-.00147)	0.00134(0.00037)	0.01845(-.00102)	0.00344(-.00089)	0.03059(0.00338)	0.0248	0.0241
O(3)	0.01796(0.00254)	-0.00001(-.00212)	-0.00706(0.00041)	0.02749(0.00053)	-0.01324(0.00353)	0.05490(-.00706)	0.0334	0.0321
O(4)	0.04640(-.01904)	0.00060(0.00628)	-0.02464(0.00953)	0.03659(0.00020)	0.00295(-.00477)	0.03601(-.00025)	0.0397	0.0333
O(5)	0.01917(0.00155)	0.00238(-.00127)	-0.00308(0.00158)	0.01648(-.00001)	-0.00373(0.00191)	0.02139(-.00543)	0.0190	0.0177
O(6)	0.02670(0.00043)	0.00641(0.00022)	0.00092(-.00040)	0.02392(-.00196)	-0.01002(0.00393)	0.04225(0.00314)	0.0310	0.0315
O(11)	0.02928(-.00736)	0.00052(-.00002)	0.00142(-.00059)	0.01416(0.00033)	0.00321(0.00079)	0.03474(-.00004)	0.0261	0.0237
O(21)	0.02292(-.00271)	-0.00585(0.00432)	-0.00130(-.00220)	0.01914(-.00034)	-0.00004(0.00104)	0.01485(-.00145)	0.0190	0.0175
O(31)	0.02713(-.00003)	0.00060(0.00107)	0.00000(0.00363)	0.02243(0.00178)	-0.00342(0.00046)	0.01735(-.00031)	0.0223	0.0228
O(41)	0.02210(0.00447)	-0.00232(-.00011)	0.00629(0.00194)	0.02461(-.00136)	0.00780(-.00053)	0.03117(0.00122)	0.0260	0.0274
O(61)	0.03053(-.00393)	0.00299(-.00394)	0.00221(-.00245)	0.02221(-.00797)	0.00523(-.00553)	0.03707(-.00649)	0.0299	0.0238
C(1)	0.01537(0.00379)	0.00029(-.00055)	-0.00092(-.00025)	0.01623(-.00003)	-0.00066(0.00095)	0.01523(-.00232)	0.0156	0.0161
C(2)	0.01573(0.00337)	-0.00021(-.00094)	0.00158(-.00161)	0.01938(-.00109)	-0.00048(0.00032)	0.02037(0.00310)	0.0185	0.0203
C(3)	0.01766(0.00232)	0.00219(-.00214)	-0.00295(-.00280)	0.02102(0.00123)	-0.00540(-.00005)	0.02303(0.00540)	0.0206	0.0236
C(4)	0.01973(0.00143)	0.00326(0.00016)	-0.00605(-.00112)	0.02179(0.00246)	-0.00296(0.00002)	0.02385(0.00461)	0.0218	0.0246
C(5)	0.02025(0.00247)	0.00347(0.00031)	-0.00004(-.00487)	0.01945(-.00033)	-0.00015(0.00051)	0.01975(0.00167)	0.0198	0.0211
C(6)	0.02576(0.00153)	0.00323(0.00345)	-0.00129(-.00273)	0.01903(0.00098)	0.00349(-.00157)	0.03571(0.00109)	0.0268	0.0280
C(11)	0.02160(-.00108)	0.00109(-.00060)	-0.00109(-.00054)	0.01743(0.00030)	0.00747(-.00011)	0.02302(-.00080)	0.0207	0.0202
C(21)	0.01526(0.00354)	-0.00054(0.00023)	-0.00126(-.00032)	0.01322(0.00159)	0.00247(-.00008)	0.01475(-.00143)	0.0144	0.0156
C(31)	0.01574(0.00526)	0.00095(-.00077)	0.00007(0.00161)	0.01471(0.00236)	0.00133(0.00025)	0.01719(-.00034)	0.0159	0.0183
C(41)	0.01692(0.00609)	-0.00094(-.00032)	0.00022(0.00237)	0.01518(0.00240)	0.00333(0.00096)	0.01934(0.00066)	0.0171	0.0202
C(51)	0.01894(0.00221)	-0.00354(0.00056)	-0.00224(0.00013)	0.01597(0.00164)	0.00014(-.00003)	0.01981(0.00198)	0.0182	0.0202
C(61)	0.03290(-.00742)	-0.00266(-.00133)	-0.00059(-.00118)	0.01647(0.00115)	-0.00240(-.00181)	0.02903(0.00277)	0.0261	0.0250

R1 = Sum(abs(U(obs)-U(calc)))/Sum(abs(U(obs)))   =   0.16476

R2 = Sqrt(Sum((U(obs)-U(calc))**2)/Sum(U(obs)**2)) =   0.18437

S = Sqrt(Sum((U(obs)-U(calc))**2)/(6*N-NS*M))   =   0.00347

N = Number of Atoms in Rigid Group   =   23

NS = Symmetry Factor   =   1

M = Number of Rigid-Body Parameters   =   20

Largest abs(U(obs)-U(calc))   =   0.01904

TLS-Mode

```
==================================================================================================================================
Inertial Tensor I, Eigenvectors and Eigenvalues of I in the Cartesian XO,YO,ZO System and Angular Relation with X,Y,Z System
----------------------------------------------------------------------------------------------------------------------------------
               XO        YO        ZO          Value             X         Y         Z     Origin (Mass-Weighted)
----------------------------------------------------------------------------------------------------------------------------------
I(1)     -0.48007  -0.77434  -0.41223        2851.51          118.69    140.75    107.11   X =  0.23152
I(2)      0.68391  -0.03608  -0.72867        2126.25           46.85     92.07    149.70   Y =  0.36677
I(3)      0.54937  -0.63174   0.54690        1305.07           56.68    129.18     65.80   Z =  0.34598


Librational Tensor, L(rad**2)                          Eigenvectors and Eigenvalues of L in the Inertial System XI,YI,ZI
----------------------------------------------------------------------------------------------------------------------------------
                                                                  XI        YI        ZI         rad**2    deg**2
----------------------------------------------------------------------------------------------------------------------------------
0.00235(.00020)-0.00016(.00009)-0.00023(.00010)       L(1)   0.97782  -0.16587  -0.12786        0.00240      7.89
                0.00138(.00015) 0.00008(.00011)       L(2)   0.17326   0.98366   0.04901        0.00136      4.46
                                0.00056(.00011)       L(3)   0.11764  -0.07007   0.99058        0.00052      1.72


Translational Tensor, T(ang**2)                        Eigenvectors and Eigenvalues of T in the Inertial System XI,YI,ZI
----------------------------------------------------------------------------------------------------------------------------------
                                                                  XI        YI        ZI         Ang^2
----------------------------------------------------------------------------------------------------------------------------------
0.01962(.00081) 0.00039(.00073)-0.00240(.00079)       T(1)   0.96730   0.05431  -0.24774        0.02026
                0.01452(.00098) 0.00028(.00094)       T(2)  -0.03049   0.99462   0.09900        0.01454
                                0.01096(.00132)       T(3)   0.25179  -0.08821   0.96375        0.01031

Cross Tensor, S(rad*Ang)
----------------------------------------------------------------------------------------------------------------------------------
 0.00027(.00025) 0.00042(.00030) 0.00009(.00020)
-0.00071(.00015)-0.00064(.00021) 0.00082(.00015)
-0.00055(.00017)-0.00048(.00015) 0.00037(.00033)

Calculation of the Origin Shift that Symmetrizes S                      -  Trace old-T =    0.04510       Trace new-T =    0.04379
----------------------------------------------------------------------------------------------------------------------------------
Shift Origin in I                 New S-Tensor                New T-Tensor       Eigenvectors and Values of New-T in I-System
----------------------------------------------------------------------------------------------------------------------------------
Rol(1)   0.65608      0.00017  -0.00033  -0.00039      0.01912  -0.00019  -0.00191 New T(1)  0.97416 -0.07203 -0.21407      0.01955
Rol(2)  -0.11960     -0.00033  -0.00054  -0.00005     -0.00019   0.01415   0.00095 New T(2)  0.11323  0.97583  0.18691      0.01430
Rol(3)   0.35090     -0.00039  -0.00005   0.00037     -0.00191   0.00095   0.01053 New T(3)  0.19543 -0.20632  0.95877      0.00993

                    Angular Relationships (Degrees)
                    ===============================
Libration Axes    -     Inertial  Axes      Libration Axes - Crystal Axes
-------------------------------------------------------------------------
                    XI      YI      ZI                X       Y       Z
L(1)              12.09   99.55   97.35          130.78  132.10  101.36
L(2)              80.02   10.37   87.19           51.94  101.57  151.66
L(3)              83.24   94.02    7.87           63.91  135.59   64.41
```

Translation Axes - Inertial Axes	XI	YI	ZI	Translation Axes - Crystal Axes X	Y	Z
New T(1)	13.05	94.13	102.36	129.38	128.06	108.19
New T(2)	83.50	12.62	79.23	44.30	103.94	143.05
New T(3)	78.73	101.91	16.51	73.03	138.55	59.09

Rigid-Body Model Libration Corrections for Bond Distances and "Hirshfeld Rigid-Bond" Test (Acta Cryst,(1976),A32,239-244)

Bond		Bond Distance		Components of the Correction			Vibration Along the Interatomic Bond				Angle with Lib. Axes		
Atom(I)	Atom(J)	Obsd	Calcd	Del(L)	Del(M)	Del(N)	I to J	J to I	Difference	Sqrt(Diff)	L(1)	L(2)	L(3)
O(1)	- C(1)	1.4216	1.4235	0.0008	-0.0004	-0.0017	0.0156(4)	0.0159(3)	0.0003(5)	0.0171	38.04	98.15	126.85
O(1)	- C(21)	1.4286	1.4302	-0.0013	0.0001	-0.0011	0.0133(4)	0.0143(3)	0.0010(5)	0.0313	152.30	94.37	117.30
O(2)	- C(2)	1.4247	1.4267	0.0003	-0.0019	0.0002	0.0194(6)	0.0193(4)	0.0002(7)	0.0134	62.98	151.30	81.05
O(3)	- C(3)	1.4238	1.4255	-0.0012	-0.0012	-0.0002	0.0203(7)	0.0205(4)	0.0002(8)	0.0137	135.70	133.90	94.78
O(4)	- C(4)	1.4100	1.4125	-0.0007	0.0005	-0.0023	0.0177(8)	0.0187(4)	0.0010(9)	0.0320	111.88	83.24	157.00
O(5)	- C(1)	1.4108	1.4128	-0.0003	0.0019	-0.0003	0.0159(5)	0.0160(3)	0.0001(6)	0.0117	115.68	28.33	101.16
O(5)	- C(5)	1.4386	1.4410	0.0009	-0.0004	0.0023	0.0186(5)	0.0191(4)	0.0005(6)	0.0220	63.17	94.58	27.29
O(6)	- C(6)	1.4168	1.4190	-0.0005	0.0003	0.0022	0.0330(6)	0.0343(5)	0.0013(8)	0.0365	128.67	82.69	39.62
O(11)	- C(11)	1.4232	1.4254	-0.0007	-0.0016	-0.0014	0.0254(5)	0.0259(4)	0.0005(7)	0.0221	98.51	147.37	121.23
O(21)	- C(21)	1.4079	1.4102	0.0005	0.0015	0.0017	0.0152(5)	0.0157(3)	0.0005(6)	0.0224	88.67	37.20	52.84
O(21)	- C(51)	1.4450	1.4470	-0.0008	-0.0015	0.0011	0.0156(5)	0.0159(4)	0.0003(6)	0.0174	120.45	139.34	65.83
O(31)	- C(31)	1.4031	1.4056	-0.0006	-0.0008	-0.0023	0.0168(5)	0.0179(3)	0.0011(6)	0.0330	96.21	119.58	149.64
O(41)	- C(41)	1.4190	1.4205	0.0012	0.0006	-0.0010	0.0167(5)	0.0160(3)	0.0007(6)	0.0259	29.61	68.21	109.03
O(61)	- C(61)	1.4212	1.4230	-0.0012	0.0003	-0.0014	0.0315(6)	0.0323(5)	0.0008(8)	0.0284	145.04	89.21	124.95
C(1)	- C(2)	1.5346	1.5365	0.0013	0.0015	0.0003	0.0159(3)	0.0170(4)	0.0012(5)	0.0345	49.12	41.49	84.08
C(2)	- C(3)	1.5198	1.5224	0.0009	-0.0003	0.0025	0.0206(4)	0.0200(4)	0.0006(5)	0.0254	64.93	90.91	25.09
C(3)	- C(4)	1.5257	1.5278	0.0003	-0.0021	0.0002	0.0199(4)	0.0200(4)	0.0001(6)	0.0101	65.15	153.88	82.47
C(4)	- C(5)	1.5258	1.5277	-0.0013	-0.0014	-0.0003	0.0227(4)	0.0233(4)	0.0006(6)	0.0239	132.39	136.78	96.90
C(5)	- C(6)	1.5228	1.5249	0.0002	-0.0021	-0.0001	0.0178(4)	0.0186(5)	0.0008(6)	0.0289	65.00	154.98	89.08
C(11)	- C(21)	1.5241	1.5266	0.0001	-0.0019	0.0015	0.0122(4)	0.0115(3)	0.0007(5)	0.0265	80.78	143.82	55.37
C(21)	- C(31)	1.5396	1.5418	-0.0008	-0.0004	0.0021	0.0157(3)	0.0164(3)	0.0007(4)	0.0268	134.46	100.10	46.23
C(31)	- C(41)	1.5254	1.5277	-0.0003	-0.0022	0.0001	0.0150(3)	0.0148(3)	0.0002(4)	0.0125	89.15	175.75	85.84
C(41)	- C(51)	1.5248	1.5275	-0.0002	-0.0005	-0.0027	0.0207(3)	0.0198(4)	0.0008(5)	0.0290	79.02	106.24	160.22
C(51)	- C(61)	1.5135	1.5155	0.0004	-0.0020	-0.0004	0.0192(4)	0.0200(5)	0.0008(6)	0.0288	58.26	147.74	95.18

Sqrt(Sum(DelIJ**2)/Nrb) =   0.0007

- Indicates bonds exceeding the 5.0 sigma test level

Test Matrix for Rigid-Body Vibrations - /Del(A,B)/ = /Z(A,B)**2 - Z(B,A)**2/ Should be Near Zero (Acta Cryst A34,1978,828)

Atom-Atom		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1 O(1)	-	0	2	2	14	0	1	1	1	5	0	8	0	1	3	3	2	3	0	-1	1	2	2	1
2 O(2)	-	3	0	2	1	1	1	3	7	1	5	7	2	0	1	1	1	1	3	8	6	6	7	1
3 O(3)	-	4	3	0	8	0	1	10	2	3	3	11	1	1	0	3	1	3	3	2	3	5	2	7
4 O(4)	-	5	5	3	0	0	5	5	3	21	22	5	3	1	2	-1	0	0	8	14	23	23	12	1
5 O(5)	-	2	4	4	4	0	3	3	8	2	3	6	0	0	1	1	0	1	2	1	3	4	1	7
6 O(6)	-	5	6	5	4	3	0	1	6	4	1	4	3	1	1	0	0	-1	2	3	3	3	2	8
7 O(11)	-	3	3	5	7	5	8	0	1	0	2	8	4	8	9	6	2	0	0	2	3	3	2	0
8 O(21)	-	2	4	6	6	3	6	4	0	0	1	2	5	2	1	5	5	5	0	-1	1	1	0	1
9 O(31)	-	3	5	6	6	5	7	3	4	0	2	10	5	8	7	4	6	0	1	1	-1	1	0	2
10 O(41)	-	4	7	9	8	6	8	6	4	3	0	4	0	1	2	2	0	3	0	1	2	-1	2	0
11 O(61)	-	4	6	7	6	3	4	6	3	5	4	0	8	9	11	12	10	6	5	8	10	8	3	-1
12 C(1)	-	-1	2	4	4	-1	4	3	3	4	5	4	0	-1	2	1	2	2	3	0	0	1	0	6
13 C(2)	-	2	-1	2	4	2	4	4	4	5	7	5	-2	0	-1	1	0	2	4	0	1	1	1	5
14 C(3)	-	3	2	-1	2	3	4	5	5	5	7	5	3	-2	0	0	0	1	3	2	3	4	3	5
15 C(4)	-	4	4	2	-1	2	3	6	5	6	7	5	3	2	-2	0	-1	0	2	2	4	4	1	9
16 C(5)	-	3	4	4	2	-1	2	6	4	5	6	3	2	3	3	-2	0	-1	1	3	3	2	2	7
17 C(6)	-	4	6	5	3	2	-1	7	5	6	7	3	4	4	4	3	-2	0	2	5	6	6	3	7
18 C(11)	-	2	3	6	7	4	7	-1	2	3	5	5	3	4	5	6	5	6	0	-1	0	1	2	1
19 C(21)	-	-1	4	6	6	3	6	2	-1	2	4	4	2	4	4	5	4	5	-2	0	-1	1	0	2
20 C(31)	-	2	5	7	7	4	7	3	2	-1	2	4	4	5	5	6	5	6	3	-2	0	0	0	2
21 C(41)	-	3	6	7	7	4	6	5	2	2	-1	3	4	5	6	6	5	5	4	2	-2	0	-1	1
22 C(51)	-	3	6	7	7	4	6	5	-1	4	2	2	4	5	6	6	5	5	4	2	2	-2	0	-1
23 C(61)	-	4	6	8	7	4	5	6	2	5	3	-1	4	6	6	6	5	5	5	4	4	3	-2	0

Remarks

- Upper Triangle Entries Represent /Del(A,B)/*1000 Values

- Lower Triangle Entries Represent Distances (A-B) Angstrom

- Negative Entries Indicate Bonded Atoms

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==================================================================================================================================
Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)
==================================================================================================================================
    The Following Tests are done. Faults are Marked Under Note
    -- V : Valency Check Fault for H, C
    -- S : Bond Too Short
    -- A : Unusual Bond Angle Values (PLEASE CHECK)
==================================================================================================================================
 *** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE  *** (CIP Special rules NOT Implemented)
 *** See Angew.Chem.Intern. Ed. Eng.,(1966),5,385 & (1982),21,567 for Authoritative Details for Special Cases

                                                                                                  =A.N.G.L.E.S=   =B.O.N.D.S=
Atom Label  - Connected to  (May be Incomplete for Polymeric Structures)          nra min max  Aver  min   max nrb  tnr Hyb RS Note
----------------------------------------------------------------------------------------------------------------------------------
   1 O(1)   - C(1)    C(21)   ------- ------- ------- ------- ------- ------- ------- 1 114 114 114.3 1.422 1.429  2  42 sp3
   2 O(2)   - C(2)    H(23)   ------- ------- ------- ------- ------- ------- ------- 1 111 111 111.3 0.972 1.425  2  37 sp3
   3 O(3)   - C(3)    H(33)   ------- ------- ------- ------- ------- ------- ------- 1 110 110 109.9 0.960 1.424  2  34 sp3
   4 O(4)   - C(4)    H(43)   ------- ------- ------- ------- ------- ------- ------- 1 112 112 112.5 0.912 1.410  2  35 sp3
   5 O(5)   - C(1)    C(5)    ------- ------- ------- ------- ------- ------- ------- 1 116 116 116.0 1.411 1.439  2  40 sp3
   6 O(6)   - C(6)    H(63)   ------- ------- ------- ------- ------- ------- ------- 1 110 110 110.0 0.956 1.417  2  32 sp3
   7 O(11)  - C(11)   H(101)  ------- ------- ------- ------- ------- ------- ------- 1 105 105 105.0 0.974 1.423  2  38 sp3
   8 O(21)  - C(21)   C(51)   ------- ------- ------- ------- ------- ------- ------- 1 112 112 111.6 1.408 1.445  2  41 sp3
   9 O(31)  - C(31)   H(301)  ------- ------- ------- ------- ------- ------- ------- 1 109 109 109.4 0.969 1.403  2  39 sp3
  10 O(41)  - C(41)   H(401)  ------- ------- ------- ------- ------- ------- ------- 1 108 108 107.8 0.976 1.419  2  36 sp3
  11 O(61)  - C(61)   H(601)  ------- ------- ------- ------- ------- ------- ------- 1 109 109 108.5 0.972 1.421  2  33 sp3
  12 C(1)   - O(1)    O(5)    C(2)    H(1)    ------- ------- ------- ------- ------- 6 105 111 109.5 1.102 1.535  4  30 sp3  R
  13 C(2)   - O(2)    C(1)    C(3)    H(2)    ------- ------- ------- ------- ------- 6 107 111 109.5 1.106 1.535  4  26 sp3  R
  14 C(3)   - O(3)    C(2)    C(4)    H(3)    ------- ------- ------- ------- ------- 6 108 112 109.5 1.098 1.526  4  23 sp3  S
  15 C(4)   - O(4)    C(3)    C(5)    H(4)    ------- ------- ------- ------- ------- 6 106 113 109.5 1.102 1.526  4  24 sp3  S
  16 C(5)   - O(5)    C(4)    C(6)    H(5)    ------- ------- ------- ------- ------- 6 106 112 109.5 1.104 1.526  4  28 sp3  R
  17 C(6)   - O(6)    C(5)    H(6)    H(61)   ------- ------- ------- ------- ------- 6 108 112 109.5 1.083 1.523  4  20 sp3
  18 C(11)  - O(11)   C(21)   H(11)   H(12)   ------- ------- ------- ------- ------- 6 108 111 109.5 1.091 1.524  4  22 sp3
  19 C(21)  - O(1)    O(21)   C(11)   C(31)   ------- ------- ------- ------- ------- 6 105 115 109.5 1.408 1.540  4  31 sp3  S
  20 C(31)  - O(31)   C(21)   C(41)   H(31)   ------- ------- ------- ------- ------- 6 102 116 109.4 1.102 1.540  4  27 sp3  S
  21 C(41)  - O(41)   C(31)   C(51)   H(41)   ------- ------- ------- ------- ------- 6 102 112 109.4 1.097 1.525  4  25 sp3  S
  22 C(51)  - O(21)   C(41)   C(61)   H(51)   ------- ------- ------- ------- ------- 6 106 115 109.4 1.103 1.525  4  29 sp3  R
  23 C(61)  - O(61)   C(51)   H(62)   H(611)  ------- ------- ------- ------- ------- 6 107 113 109.4 1.087 1.514  4  21 sp3

  24 H(1)   - C(1)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.102 1.102  1  11
  25 H(2)   - C(2)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.106 1.106  1   6
  26 H(3)   - C(3)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.098 1.098  1   3
  27 H(4)   - C(4)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.102 1.102  1   4
  28 H(5)   - C(5)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.104 1.104  1   9
  29 H(6)   - C(6)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.083 1.083  1   1
  30 H(11)  - C(11)   ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.091 1.091  1   7
  31 H(12)  - C(11)   ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.095 1.095  1   7
  32 H(23)  - O(2)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 0.972 0.972  1  18
  33 H(31)  - C(31)   ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.102 1.102  1   8
  34 H(33)  - O(3)    ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 0.960 0.960  1  15
  35 H(41)  - C(41)   ------- ------- ------- ------- ------- ------- ------- ------- 0   0   0   0.0 1.097 1.097  1   5
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36	H(43)	- O(4)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.912	0.912	1	16
37	H(51)	- C(51)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.103	1.103	1	10
38	H(61)	- C(6)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.090	1.090	1	1
39	H(62)	- C(61)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.087	1.087	1	2
40	H(63)	- O(6)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.956	0.956	1	12
41	H(101)	- O(11)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.974	0.974	1	14

42	H(301) - O(31)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.969	0.969	1	19
43	H(401) - O(41)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.976	0.976	1	17
44	H(601) - O(61)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.972	0.972	1	13
45	H(611) - C(61)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.092	1.092	1	2

Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: d(i-j) < R(i) + R(j) + Tol

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances
-- The Bond Distance and Angle esd’s have been Incremented to Include the Effect of the Unit-cell esd.
(Rel.Error in Dist. 0.0001 Ang. , Abs. Angle Error 0.006 Deg.)

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - esd in last digit in ().

O(1) - C(1)	1.4216(13)	O(1) - C(21)	1.4286(17)	O(2) - C(2)	1.4247(16)	O(3) - C(3)	1.424(2)
O(4) - C(4)	1.410(2)	O(5) - C(1)	1.4108(14)	O(5) - C(5)	1.4386(19)	O(6) - C(6)	1.4168(19)
O(11) - C(11)	1.4232(19)	O(21) - C(21)	1.4079(16)	O(21) - C(51)	1.4450(14)	O(31) - C(31)	1.4031(18)
O(41) - C(41)	1.4190(16)	O(61) - C(61)	1.421(2)	C(1) - C(2)	1.5346(13)	C(2) - C(3)	1.5198(18)
C(3) - C(4)	1.5257(15)	C(4) - C(5)	1.5258(17)	C(5) - C(6)	1.5228(15)	C(11) - C(21)	1.5241(13)
C(21) - C(31)	1.5396(12)	C(31) - C(41)	1.5254(13)	C(41) - C(51)	1.5248(16)	C(51) - C(61)	1.5135(15)
O(2) > H(23)	0.972(3)	O(3) > H(33)	0.960(4)	O(4) - H(43)	0.912(4)	O(6) > H(63)	0.956(4)
O(11) > H(101)	0.974(3)	O(31) > H(301)	0.969(3)	O(41) > H(401)	0.976(3)	O(61) > H(601)	0.972(3)
C(1) > H(1)	1.102(3)	C(2) > H(2)	1.106(2)	C(3) > H(3)	1.098(2)	C(4) > H(4)	1.102(2)
C(5) > H(5)	1.104(2)	C(6) > H(6)	1.083(4)	C(6) > H(61)	1.090(4)	C(11) > H(11)	1.091(3)
C(11) > H(12)	1.095(3)	C(31) > H(31)	1.102(3)	C(41) > H(41)	1.097(3)	C(51) > H(51)	1.103(3)
C(61) > H(62)	1.087(3)	C(61) > H(611)	1.092(4)				

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - esd in last digit in ().

C(1) - O(1) - C(21)	114.30(9)	C(1) - O(5) - C(5)	115.96(9)	C(21) - O(21) - C(51)	111.64(9)
O(1) - C(1) - O(5)	110.49(9)	O(1) - C(1) - C(2)	110.33(8)	O(5) - C(1) - C(2)	110.84(7)
O(2) - C(2) - C(1)	110.10(10)	O(2) - C(2) - C(3)	110.33(10)	C(1) - C(2) - C(3)	111.02(7)
O(3) - C(3) - C(2)	111.57(10)	O(3) - C(3) - C(4)	108.12(11)	C(2) - C(3) - C(4)	108.13(9)
O(4) - C(4) - C(3)	112.52(12)	O(4) - C(4) - C(5)	106.02(10)	C(3) - C(4) - C(5)	110.81(10)
O(5) - C(5) - C(4)	110.66(9)	O(5) - C(5) - C(6)	106.10(10)	C(4) - C(5) - C(6)	111.94(10)
O(6) - C(6) - C(5)	111.53(10)	O(11) - C(11) - C(21)	111.19(11)	O(1) - C(21) - O(21)	111.00(9)
O(1) - C(21) - C(11)	109.93(8)	O(1) - C(21) - C(31)	108.43(9)	O(21) - C(21) - C(11)	107.21(9)
O(21) - C(21) - C(31)	105.18(8)	C(11) - C(21) - C(31)	115.00(8)	O(31) - C(31) - C(21)	115.76(10)
O(31) - C(31) - C(41)	115.35(10)	C(21) - C(31) - C(41)	102.40(7)	O(41) - C(41) - C(31)	112.39(9)
O(41) - C(41) - C(51)	111.63(11)	C(31) - C(41) - C(51)	102.32(7)	O(21) - C(51) - C(41)	105.64(9)
O(21) - C(51) - C(61)	109.75(9)	C(41) - C(51) - C(61)	114.94(9)	O(61) - C(61) - C(51)	113.02(12)
C(2) - O(2) - H(23)	111.3(2)	C(3) - O(3) - H(33)	109.9(2)	C(4) - O(4) - H(43)	112.5(3)
C(6) - O(6) - H(63)	110.0(3)	C(11) - O(11) - H(101)	105.0(2)	C(31) - O(31) - H(301)	109.45(18)
C(41) - O(41) - H(401)	107.8(2)	C(61) - O(61) - H(601)	108.5(2)	O(1) - C(1) - H(1)	110.24(14)
O(5) - C(1) - H(1)	105.20(14)	C(2) - C(1) - H(1)	109.63(14)	O(2) - C(2) - H(2)	109.88(15)
C(1) - C(2) - H(2)	106.80(15)	C(3) - C(2) - H(2)	108.63(17)	O(3) - C(3) - H(3)	109.74(17)
C(2) - C(3) - H(3)	109.77(17)	C(4) - C(3) - H(3)	109.47(15)	O(4) - C(4) - H(4)	110.23(18)
C(3) - C(4) - H(4)	107.92(15)	C(5) - C(4) - H(4)	109.32(16)	O(5) - C(5) - H(5)	109.82(17)
C(4) - C(5) - H(5)	108.87(16)	C(6) - C(5) - H(5)	109.41(14)	O(6) - C(6) - H(6)	107.9(2)
O(6) - C(6) - H(61)	110.2(2)	C(5) - C(6) - H(6)	109.1(2)	C(5) - C(6) - H(61)	109.9(2)
H(6) - C(6) - H(61)	108.2(3)	O(11) - C(11) - H(11)	108.0(2)	O(11) - C(11) - H(12)	110.98(17)
C(21) - C(11) - H(11)	109.75(18)	C(21) - C(11) - H(12)	108.98(15)	H(11) - C(11) - H(12)	107.8(3)

O(31)	-	C(31)	-	H(31)	106.62(15)		C(21)	-	C(31)	-	H(31)	108.34(15)		C(41)	-	C(31)	-	H(31)	108.03(15)
O(41)	-	C(41)	-	H(41)	110.85(15)		C(31)	-	C(41)	-	H(41)	109.11(16)		C(51)	-	C(41)	-	H(41)	110.22(15)
O(21)	-	C(51)	-	H(51)	107.80(15)		C(41)	-	C(51)	-	H(51)	110.15(18)		C(61)	-	C(51)	-	H(51)	108.33(19)
O(61)	-	C(61)	-	H(62)	107.3(2)		O(61)	-	C(61)	-	H(611)	111.0(2)		C(51)	-	C(61)	-	H(62)	108.8(2)
C(51)	-	C(61)	-	H(611)	108.9(2)		H(62)	-	C(61)	-	H(611)	107.6(3)							

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Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)

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O(5)	C(1)	O(1)	C(21)	107.82(9)	C(2)	C(1)	O(1)	C(21)	-129.26(8)	O(1)	C(1)	O(5)	C(5)	67.72(11)
C(2)	C(1)	O(5)	C(5)	-54.91(12)	O(1)	C(1)	C(2)	O(2)	54.75(11)	O(1)	C(1)	C(2)	C(3)	-67.73(10)
O(5)	C(1)	C(2)	O(2)	177.47(10)	O(5)	C(1)	C(2)	C(3)	54.99(11)	O(2)	C(2)	C(3)	O(3)	62.85(13)
O(2)	C(2)	C(3)	C(4)	-178.38(9)	C(1)	C(2)	C(3)	O(3)	-174.80(9)	C(1)	C(2)	C(3)	C(4)	-56.03(11)
O(3)	C(3)	C(4)	O(4)	-64.29(14)	O(3)	C(3)	C(4)	C(5)	177.21(10)	C(2)	C(3)	C(4)	O(4)	174.77(11)
C(2)	C(3)	C(4)	C(5)	56.27(11)	O(4)	C(4)	C(5)	O(5)	-177.24(12)	O(4)	C(4)	C(5)	C(6)	64.63(14)
C(3)	C(4)	C(5)	O(5)	-54.87(12)	C(3)	C(4)	C(5)	C(6)	-173.00(10)	C(4)	C(5)	O(5)	C(1)	55.16(12)
C(6)	C(5)	O(5)	C(1)	176.79(9)	O(5)	C(5)	C(6)	O(6)	-56.44(15)	C(4)	C(5)	C(6)	O(6)	64.37(15)
O(11)	C(11)	C(21)	O(1)	50.61(12)	O(11)	C(11)	C(21)	O(21)	171.37(10)	O(11)	C(11)	C(21)	C(31)	-72.09(13)
O(21)	C(21)	O(1)	C(1)	-44.75(11)	C(11)	C(21)	O(1)	C(1)	73.70(11)	C(31)	C(21)	O(1)	C(1)	-159.81(8)
O(1)	C(21)	O(21)	C(51)	-102.42(11)	C(11)	C(21)	O(21)	C(51)	137.50(10)	C(31)	C(21)	O(21)	C(51)	14.66(13)
O(1)	C(21)	C(31)	O(31)	-38.73(12)	O(1)	C(21)	C(31)	C(41)	87.62(10)	O(21)	C(21)	C(31)	O(31)	-157.54(10)
O(21)	C(21)	C(31)	C(41)	-31.18(12)	C(11)	C(21)	C(31)	O(31)	84.77(13)	C(11)	C(21)	C(31)	C(41)	-148.88(10)
O(31)	C(31)	C(41)	O(41)	-78.47(15)	O(31)	C(31)	C(41)	C(51)	161.66(10)	C(21)	C(31)	C(41)	O(41)	154.91(11)
C(21)	C(31)	C(41)	C(51)	35.04(12)	O(41)	C(41)	C(51)	O(21)	-147.67(10)	O(41)	C(41)	C(51)	C(61)	91.19(12)
C(31)	C(41)	C(51)	O(21)	-27.26(12)	C(31)	C(41)	C(51)	C(61)	-148.41(10)	C(41)	C(51)	O(21)	C(21)	8.06(14)
C(61)	C(51)	O(21)	C(21)	132.52(11)	O(21)	C(51)	C(61)	O(61)	-69.55(13)	C(41)	C(51)	C(61)	O(61)	49.32(13)

H(1)	C(1)	O(1)	C(21)	-8.03(17)	H(1)	C(1)	O(5)	C(5)	-173.32(15)	O(1)	C(1)	C(2)	H(2)	174.01(16)
O(5)	C(1)	C(2)	H(2)	-63.28(17)	H(1)	C(1)	C(2)	O(2)	-66.84(17)	H(1)	C(1)	C(2)	C(3)	170.68(14)
H(1)	C(1)	C(2)	H(2)	52.4(2)	C(1)	C(2)	O(2)	H(23)	93.3(2)	C(3)	C(2)	O(2)	H(23)	-143.8(2)
H(2)	C(2)	O(2)	H(23)	-24.1(3)	O(2)	C(2)	C(3)	H(3)	-59.01(17)	C(1)	C(2)	C(3)	H(3)	63.33(16)
H(2)	C(2)	C(3)	O(3)	-57.65(17)	H(2)	C(2)	C(3)	C(4)	61.12(16)	H(2)	C(2)	C(3)	H(3)	-179.51(19)
C(2)	C(3)	O(3)	H(33)	-91.4(3)	C(4)	C(3)	O(3)	H(33)	149.8(2)	H(3)	C(3)	O(3)	H(33)	30.4(3)
O(3)	C(3)	C(4)	H(4)	57.5(2)	C(2)	C(3)	C(4)	H(4)	-63.40(19)	H(3)	C(3)	C(4)	O(4)	55.2(2)
H(3)	C(3)	C(4)	C(5)	-63.28(19)	H(3)	C(3)	C(4)	H(4)	177.1(2)	C(3)	C(4)	O(4)	H(43)	47.9(5)
C(5)	C(4)	O(4)	H(43)	169.2(5)	H(4)	C(4)	O(4)	H(43)	-72.6(5)	O(4)	C(4)	C(5)	H(5)	-56.45(19)
C(3)	C(4)	C(5)	H(5)	65.92(18)	H(4)	C(4)	C(5)	O(5)	63.95(18)	H(4)	C(4)	C(5)	C(6)	-54.18(19)
H(4)	C(4)	C(5)	H(5)	-175.3(2)	H(5)	C(5)	O(5)	C(1)	-65.06(18)	O(5)	C(5)	C(6)	H(6)	-175.5(2)
O(5)	C(5)	C(6)	H(61)	66.0(2)	C(4)	C(5)	C(6)	H(6)	-54.7(2)	C(4)	C(5)	C(6)	H(61)	-173.1(2)
H(5)	C(5)	C(6)	O(6)	-174.86(19)	H(5)	C(5)	C(6)	H(6)	66.1(3)	H(5)	C(5)	C(6)	H(61)	-52.4(3)
C(5)	C(6)	O(6)	H(63)	86.8(3)	H(6)	C(6)	O(6)	H(63)	-153.4(3)	H(61)	C(6)	O(6)	H(63)	-35.5(4)
C(21)	C(11)	O(11)	H(101)	-67.55(19)	H(11)	C(11)	O(11)	H(101)	172.0(2)	H(12)	C(11)	O(11)	H(101)	53.9(3)
H(11)	C(11)	C(21)	O(1)	170.1(2)	H(11)	C(11)	C(21)	O(21)	-69.1(2)	H(11)	C(11)	C(21)	C(31)	47.4(2)
H(12)	C(11)	C(21)	O(1)	-72.0(2)	H(12)	C(11)	C(21)	O(21)	48.7(2)	H(12)	C(11)	C(21)	C(31)	165.3(2)
O(1)	C(21)	C(31)	H(31)	-158.37(15)	O(21)	C(21)	C(31)	H(31)	82.82(16)	C(11)	C(21)	C(31)	H(31)	-34.88(18)
C(21)	C(31)	O(31)	H(301)	67.03(19)	C(41)	C(31)	O(31)	H(301)	-52.5(2)	H(31)	C(31)	O(31)	H(301)	-172.4(2)
O(31)	C(31)	C(41)	H(41)	44.90(17)	C(21)	C(31)	C(41)	H(41)	-81.71(16)	H(31)	C(31)	C(41)	O(41)	40.68(18)
H(31)	C(31)	C(41)	C(51)	-79.19(16)	H(31)	C(31)	C(41)	H(41)	164.06(19)	C(31)	C(41)	O(41)	H(401)	134.3(2)
C(51)	C(41)	O(41)	H(401)	-111.4(2)	H(41)	C(41)	O(41)	H(401)	11.9(3)	O(41)	C(41)	C(51)	H(51)	-31.51(18)
C(31)	C(41)	C(51)	H(51)	88.89(17)	H(41)	C(41)	C(51)	O(21)	88.69(16)	H(41)	C(41)	C(51)	C(61)	-32.46(18)
H(41)	C(41)	C(51)	H(51)	-155.2(2)	H(51)	C(51)	O(21)	C(21)	-109.7(2)	O(21)	C(51)	C(61)	H(62)	171.3(2)
O(21)	C(51)	C(61)	H(611)	54.3(2)	C(41)	C(51)	C(61)	H(62)	-69.8(2)	C(41)	C(51)	C(61)	H(611)	173.1(2)
H(51)	C(51)	C(61)	O(61)	172.99(16)	H(51)	C(51)	C(61)	H(62)	53.9(3)	H(51)	C(51)	C(61)	H(611)	-63.2(3)
C(51)	C(61)	O(61)	H(601)	59.5(3)	H(62)	C(61)	O(61)	H(601)	179.5(3)	H(611)	C(61)	O(61)	H(601)	-63.2(3)

Statistics of Bond Length per Bond Type (NOTE: A Indicates 10 Occurrences, B Indicates 11, Etc. and * more than 35)

```
Bond Type    Nr    d(min)    d(max)     d(av)  Sumrad Note  0.0       0.5       1.0       1.5       2.0       2.5       3.0 Angstrom
----------------------------------------------------------   I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I-I
 O  --  C4   14    1.4031    1.4450    1.4210    1.36        ............................B3........................................
 C4 --  C4   10    1.5135    1.5396    1.5256    1.36        ..............................55......................................
 O  --  H     8    0.9120    0.9760    0.9614    0.91        ..................161.................................................
 C  --  H    14    1.0830    1.1060    1.0966    0.91        ......................E...............................................
```

Selected Bond Lengths (Angstrom) - see Ladd & Palmer, Structure Determination by X-Ray Crystallography (1985)

```
                                                  Formal single bonds
                                                  -------------------
C4-C4 1.54   C4-C3 1.52   C4-C2 1.46   C4-N3 1.47   C4-N2 1.47   C4-O2 1.43   C3-C3 1.46   C3-C2 1.45   C3-N3 1.40   C3-N2 1.40
C3-O2 1.36   C2-C2 1.38   C2-N3 1.33   C2-N2 1.33   C2-O2 1.36   N3-N3 1.45   N3-N2 1.45   N3-O2 1.36   N2-N2 1.45   N2-O2 1.41

                                                  Formal double bonds
                                                  -------------------
C3-C3 1.34   C3-C2 1.31   C3-N2 1.32   C3-O1 1.22   C2-C2 1.28   C2-N2 1.32   C2-O1 1.16   N3-O1 1.24   N2-N2 1.25   N2-O1 1.21

Formal triple bonds                 Aromatic bonds
-------------------                 --------------
C2-C2 1.20   C2-N1 1.16   C3-C3 1.40   C2-N2 1.34   N2-N2 1.35
```

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19;
J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.

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=====================================================================================================================================
Automatic Search for Rings (3 to 24-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)
-------------------------------------------------------------------------------------------------------------------------------------

Least-Squares Planes - P*X+Q*Y+R*Z=S   ::  First Line Orthogonal(XO,YO,ZO), Second Line Fractional(X,Y,Z)
====================================        Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms
                                            Sigref - R.M.S-Error of the Contributing Atoms
  The Deviation D of an Atom with           Sigpln - Sqrt(Sum(j=1:N)(D(j)**2/(N-3))
                                            Chisq  - Chi-Squared = Sum(j=1:N)(D(j)**2)/Sigref**2
  Fractional Coordinates X,Y,Z may be       Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

  Calculated via Substitution in
                                            **** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed
  D = P*X + Q*Y + R*Z - S (2nd Line)        Note - Weights : UNIT
                                                 - Deviations from planes are in Angstrom Units
                                                 - The Plane determining Atoms have been Marked #
-------------------------------------------------------------------------------------------------------------------------------------
Nr  1        P             Q             R             S     Sigref  0.001     Sigpln  0.249     Chisq  109212.1    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------------
Ring     0.4950(6)     0.8594(3)    -0.1281(6)    1.2887(13) #O(21)  -0.019(1) #C(21)   0.147(1) #C(31)  -0.216(1) #C(41)   0.205(1)
A  5      5.377(6)      7.481(3)     -1.829(5)    1.2887(13) #C(51)  -0.117(1)  O(11)  -0.501(2)  O(31)   0.318(1)  O(41)  -0.512(2)
                                                              C(11)  -0.749(1)  C(61)   0.794(1)
-------------------------------------------------------------------------------------------------------------------------------------
Nr  2        P             Q             R             S     Sigref  0.001     Sigpln  0.321     Chisq  261896.5    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------------
Ring     0.8502(2)    -0.0482(5)     0.5243(4)      4.032(2) #O(5)    0.201(1) #C(1)   -0.209(1) #C(2)    0.237(1) #C(3)   -0.259(1)
A  6      9.236(3)     -0.419(4)      2.487(3)      4.032(2) #C(4)    0.240(1) #C(5)   -0.211(1)  O(2)   -0.235(1)  O(3)    0.247(1)
                                                              O(4)   -0.266(2)  O(21)  -1.328(1)  O(61)  -1.016(1)  C(6)    0.413(1)
                                                              C(61)  -1.278(1)
-------------------------------------------------------------------------------------------------------------------------------------
Nr  3        P             Q             R             S     Sigref  0.001     Sigpln  0.992     Chisq  999999.9    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------------
Resd     0.5617(2)    -0.6243(1)     0.5429(2)     0.5193(7) #O(1)   -0.130(1) #O(2)    0.854(1) #O(3)   -0.504(2) #O(4)   -1.700(2)
A 23      6.102(2)   -5.4344(10)    3.1291(15)     0.5193(7) #O(5)    0.769(1) #O(6)    0.961(2) #O(11)   0.329(1) #O(21)   1.249(1)
                                                             #O(31)  -2.056(1) #O(41)  -1.456(1) #O(61)   0.305(2) #C(1)    0.881(1)
                                                             #C(2)    0.798(1) #C(3)   -0.471(1) #C(4)   -0.500(1) #C(5)   -0.398(1)
                                                             #C(6)   -0.252(1) #C(11)   1.098(1) #C(21)   0.348(1) #C(31)  -0.840(1)
                                                             #C(41)  -0.858(1) #C(51)   0.626(1) #C(61)   0.947(1)
-------------------------------------------------------------------------------------------------------------------------------------
Nr  4        P             Q             R             S     Sigref  0.001     Sigpln  0.037     Chisq    1135.9    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------------
Plan    0.4983(10)    0.3621(11)     0.7877(3)    5.1986(18) #O(5)   -0.023(1) #C(1)    0.020(1) #C(5)   -0.014(1) #C(6)    0.017(1)
A  4     5.414(11)     3.152(10)      5.090(3)    5.1986(18)  O(1)   -1.185(1)  O(2)    1.223(1)  O(4)    1.069(2)  O(6)    1.125(2)
                                                              O(11)  -1.131(1)  C(2)    1.227(1)  C(3)    1.227(1)  C(4)    1.191(1)
                                                              C(11)  -1.460(1)
-------------------------------------------------------------------------------------------------------------------------------------
Nr  5        P             Q             R             S     Sigref  0.001     Sigpln  0.029     Chisq     662.5    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------------
Plan     0.6251(8)   -0.5489(10)     0.5549(4)      1.817(6) #O(2)   -0.015(1) #O(5)   -0.015(1) #C(1)    0.015(1) #C(2)    0.014(1)
A  4      6.791(8)     -4.778(9)      3.109(3)      1.817(6)  O(1)   -1.090(1)  O(3)   -1.113(2)  O(6)    0.416(2)  O(11)  -0.806(1)
```

					O(21)	0.153(1)	O(61)	-0.612(1)	C(3)	-1.166(1)	C(4)	-1.109(1)
					C(5)	-1.092(1)	C(6)	-0.864(1)	C(11)	-0.053(1)	C(21)	-0.745(1)
					C(51)	-0.512(1)	C(61)	-0.099(1)				
Nr 6	P	Q	R	S	Sigref	0.001	Sigpln	0.020	Chisq	269.0	Pl.Hyp.	P<5
Plan	0.5091(10)	0.3601(10)	0.7817(3)	6.403(3)	#O(2)	-0.010(1)	#C(2)	0.011(1)	#C(3)	0.009(1)	#C(4)	-0.009(1)

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========================================================================================================================================
A  4     5.531(11)      3.134(8)      5.026(3)      6.403(3)  O(3)    1.177(2)  O(4)    -0.131(2)  O(5)    -1.214(1)  O(6)    -0.039(2)
                                                              C(1)   -1.187(1)  C(5)    -1.204(1)  C(6)    -1.155(1)
----------------------------------------------------------------------------------------------------------------------------------------
Nr  7        P             Q             R             S     Sigref  0.001     Sigpln  0.034     Chisq     729.8    Pl.Hyp.    P<5
----------------------------------------------------------------------------------------------------------------------------------------
Plan    0.5901(11)   -0.5781(11)     0.5636(4)      0.469(9) #O(3)    0.017(2) #C(3)    -0.017(1) #C(4)    -0.017(1) #C(5)    0.016(1)
A  4     6.410(12)    -5.032(10)      3.236(4)      0.469(9)  O(1)    0.155(1)  O(2)     1.231(1)  O(4)    -1.177(2)  O(5)    1.135(1)
                                                              O(6)    1.440(2)  O(11)    0.550(1)  O(21)    1.437(1)  O(41)  -1.383(1)
                                                              O(61)   0.556(2)  C(1)     1.220(1)  C(2)     1.204(1)  C(6)    0.189(1)
                                                              C(11)   1.292(1)  C(21)    0.554(1)  C(31)   -0.687(1)  C(41)  -0.714(1)
                                                              C(51)   0.769(1)  C(61)    1.124(1)
----------------------------------------------------------------------------------------------------------------------------------------
Nr  8        P             Q             R             S     Sigref  0.001     Sigpln  0.032     Chisq     581.4    Pl.Hyp.    P<5
----------------------------------------------------------------------------------------------------------------------------------------
Plan     0.9968(1)     0.0793(6)    0.0076(15)      3.759(4) #O(4)   -0.016(2) #O(5)    -0.016(1) #C(4)     0.015(1) #C(5)    0.018(1)
A  4    10.8287(5)      0.691(5)    -1.675(11)      3.759(4)  O(3)   -1.084(1)  O(61)   -0.127(1)  C(1)    -1.079(1)  C(2)   -1.112(1)
                                                              C(3)   -1.173(1)  C(6)     1.281(1)  C(61)   -0.648(1)

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)
----------------------------------------------------------------------------------------------------------------------------------------
 1, 2=   71.80(6)   1, 3=   70.85(6)   1, 4=  62.81(10)   1, 5=   76.51(9)   1, 6=  62.53(10)   1, 7=  73.92(11)   1, 8=  55.90(11)
 2, 3=   37.60(4)   2, 4=  34.99(10)   2, 5=   31.91(9)   2, 6=   34.37(9)   2, 7=  34.41(10)   2, 8=  32.04(10)   3, 4=   61.21(9)
 3, 5=    5.69(8)   3, 6=   60.95(8)   3, 7=    3.33(9)   3, 8=   59.04(9)   4, 5=  56.64(12)   4, 6=   0.72(12)   4, 7=  58.08(13)
 4, 8=  57.89(13)   5, 6=  56.33(11)   5, 7=   2.66(12)   5, 8=  54.28(12)   6, 7=  57.80(12)   6, 8=  57.18(12)   7, 8=  56.86(13)


(Acute) Angles (Degrees) Between Axes, Lines, Bonds and L.S.-Plane
----------------------------------------------------------------------------------------------------------------------------------------
 Bond  /  Plane NM --> M      1          2          3          4          5          6          7          8          9         10
----------------------------------------------------------------------------------------------------------------------------------------
Axes O --->a  / 0M =    29.67(5),  58.23(4),  34.17(2),  29.89(9),  38.69(8),  30.61(8),  36.16(9),  85.43(9),
           b  / 0M =    59.25(5),   2.76(4),  38.63(2),  21.23(9),  33.29(8),  21.10(8),  35.31(9),   4.55(9),
           c  / 0M =    13.63(5),  18.69(4),  23.79(2),  41.00(9),  23.62(8),  40.38(8),  24.65(9),  12.47(9),
           a* / 0M =    26.98(5),  71.09(4),  41.99(2),  41.46(9),  47.19(8),  42.17(8),  44.53(9),  76.70(9),
           b* / 0M =    59.25(5),   2.76(4),  38.63(2),  21.23(9),  33.29(8),  21.10(8),  35.31(9),   4.55(9),
           c* / 0M =     7.36(5),  31.62(4),  32.88(2),  51.98(9),  33.70(8),  51.42(8),  34.31(9),   0.44(9),
O(1)  -C(1)   / 0M =    25.22(7),  82.91(6),  45.31(6), 57.96(10),  51.00(9), 58.64(10), 48.51(11), 60.71(11),
      -C(21)  / 0M =    72.28(9),  17.34(8),  19.53(7), 36.72(11), 13.97(10), 36.79(11), 16.21(11), 23.81(11),
O(2)  -C(2)   / 0M =    41.50(8),  19.36(7),   2.26(7),  0.18(11),  1.16(10),  0.84(10),  1.08(11), 51.36(11),
O(3)  -C(3)   / 0M =   29.38(10),  20.81(9),   1.31(8), 55.69(12),  2.13(11), 55.11(11),  1.36(12),  3.60(12),
O(4)  -C(4)   / 0M =   50.75(10),  21.04(9),  58.33(8),  4.95(12), 52.71(11),  4.95(11), 55.31(12),  1.26(12),
O(5)  -C(1)   / 0M =    41.53(8),  16.91(7),   4.57(6),  1.74(10),  1.21(10),  1.10(10),  3.43(11), 48.89(11),
      -C(5)   / 0M =    54.90(9),  16.64(8),  54.19(8),  0.38(12), 48.51(11),  0.38(11), 51.04(12),  1.34(12),
O(6)  -C(6)   / 0M =    11.78(9),  83.52(8),  58.87(8), 51.43(12), 64.56(11), 51.98(11), 62.06(12), 54.52(12),
O(11) -C(11)  / 0M =    10.03(9),  21.61(8),  32.74(8), 13.35(12), 31.94(11), 12.72(11), 31.41(12), 36.49(12),
O(21) -C(21)  / 0M =     6.77(8),  30.65(7),  39.81(7),  4.33(11), 39.65(10),  3.70(10), 38.85(11), 43.54(11),
      -C(51)  / 0M =     3.87(8),  32.72(7),  25.55(6), 59.88(10), 27.44(10), 59.23(10), 27.52(11),  3.82(11),
O(31) -C(31)  / 0M =    22.38(9),  36.05(8),  60.06(8),  3.67(11), 57.86(11),  4.13(11), 58.07(12), 33.31(12),
O(41) -C(41)  / 0M =    30.36(8),  52.31(7),  24.96(7), 86.11(11), 29.59(10), 85.90(10), 28.11(11), 31.36(11),
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O(61) -C(61)  / 0M =   75.99(10),  10.63(9),  26.81(8), 27.71(12), 21.16(11), 27.80(11), 23.54(12), 21.50(12),
C(1)  -C(2)   / 0M =    25.76(7),  16.90(6),   3.10(5), 51.89(10),   0.02(9),  51.27(9),  0.60(10),  1.21(10),
C(2)  -C(3)   / 0M =    51.96(9),  19.04(8),  56.64(7),  0.00(11), 50.95(10),  0.06(11), 53.41(11),  2.32(11),
C(3)  -C(4)   / 0M =    38.82(8),  19.10(7),   1.08(6),  1.35(10),  2.15(10),  0.69(10),  0.03(11), 51.14(11),
C(4)  -C(5)   / 0M =    27.65(8),  17.20(7),   3.84(7), 52.14(11),  0.61(10), 51.54(10),  1.27(11),  0.10(11),
C(5)  -C(6)   / 0M =    35.25(8),  24.20(7),   5.50(6),  1.15(10),  8.64(10),  1.84(10),  6.49(11), 56.07(11),
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C(11) -C(21)  / 0M =    35.98(7),   9.92(6),  29.50(5), 22.37(10),  27.00(9),  21.85(9), 28.96(10), 21.86(10),
C(21) -C(31)  / 0M =    13.63(7),  72.16(6),  50.48(5), 67.77(10),  55.36(9),  68.15(9), 53.71(10), 41.15(10),
C(31) -C(41)  / 0M =    16.03(7),   5.42(6),   0.67(5), 22.32(10),   0.34(9),  21.62(9),  1.01(10), 35.01(10),
C(41) -C(51)  / 0M =    12.20(8),  55.61(7),  76.66(6), 25.17(11), 77.75(10), 25.59(10), 76.66(11), 41.57(11),
C(51) -C(61)  / 0M =    37.02(8),  33.28(7),  12.23(6),  9.86(10), 15.86(10), 10.55(10), 13.56(11), 65.23(11),
```

Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

	Symmetrical Forms	References
5-Membered Rings :	E : Envelope - Phi = k X 36	D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97,(1975),1354-1358
	T : Half Chair- Phi = k X 36 + 18	
6-Membered Rings :	C : Chair - Th = 0.0	J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320
	H : Half-Chair- Th = 50.8; Phi = k X 60 + 30	
	E : Envelope - Th = 54.7; Phi = k X 60	
	S : Screw-Boat- Th = 67.5; Phi = k X 60 + 30	
	B : Boat - Th = 90.0; Phi = k X 60	
	T : Twist-Boat- Th = 90.0; Phi = k X 60 + 30	

Definitions (All Values Rounded on Esd)

Dev - Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
Cs(I),C2(I) - Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al.,Topics in Stereochemistry,V-9, (1976) pp.271-383)
Cs(I-J),C2(I-J)- Asymmetry Parameters for Bond I-J
Tors(I-J) - Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Torsion Angle Range	Full Descriptor	Short Descriptor
0 TO 30 Deg	+ Syn-Periplanar	+sp
30 to 90	+ Syn-Clinal	+sc
90 to 150	+ Anti-Clinal	+ac
150 to 180	+ Anti-Periplanar	+ap
0 to -30	- Syn-Periplanar	-sp
-30 to -90	- Syn-Clinal	-sc
-90 to -150	- Anti-Clinal	-ac
-150 to -180	- Anti-Periplanar	-ap

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

Angle Range of Subst.	Full Descriptor	Short Descriptor
0 TO 30 Deg.	Axial	ax
30 to 60	Bisectional	bi
60 to 90	Equatorial	eq

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
- The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
- Use TRNS Instructions to Obtain the Required Absolute Configuration.
- The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
- Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)

For Correct Usage of C&P Puckering Parameters see also: D. Cremer, Acta Cryst. (1984). B40, 498-500.

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==================================================================================================================================
Hexafuranose Nomencl.    O5           C2           C3           C4           C5         (IUPAC-IUB: Eur.J.Biochem. (1983), 131, 5-7)
  5-Membered Ring ( 1)   O(21)  -->   C(21)  -->   C(31)  -->   C(41)  -->   C(51)  -->
----------------------------------------------------------------------------------------------------------------------------------
Dev. (Ang)            -0.0187(13)   0.1458(11)  -0.2172(11)   0.2056(12)  -0.1155(12)
Cs(I)-Asym-Par (Deg)    44.34(12)    32.64(13)     9.32(12)    17.25(13)    37.67(13)
C2(I)-Asym-Par (Deg)     5.43(13)    37.61(13)    55.42(12)    52.06(12)    28.83(13)
Ring Bond Angle(Deg)    111.64(9)    105.18(8)    102.40(7)    102.32(7)    105.64(9)

Tors(I-J) (Deg)              14.66(13)   -31.18(12)    35.04(12)   -27.26(12)     8.06(14)
Cs(I-J)-Asym-Par   (Deg)     17.25(13)    37.67(13)    44.34(12)    32.64(13)     9.32(12)
C2(I-J)-Asym-Par   (Deg)     52.06(12)    28.83(13)     5.43(13)    37.61(13)    55.42(12)
Ring Bond Distance (Ang)    1.4079(16)   1.5396(12)   1.5254(13)   1.5248(16)   1.4450(14)

Weighted Average Ring Bond Distance = 1.4954(  6,251) Ang.  -  NOTE: 1st esd. Internal, 2nd esd External
Weighted Average Abs. Torsion Angl. =  24.39(  6,492) Deg.           see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234

Cremer & Pople Puckering Parameters  [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]
----------------------------------------------------------------------------------------------------------------------------------
Q(2)  =       0.353(1) Ang.,  Phi(2) =    265.19(19) Deg

*** NOTE *** - A Change of the Absolute Configuration Transforms Phi(2) into 180 + Phi(2).
             - A Cyclic Forward Shift of the Pivot Atom From At1 to At2 Transforms Phi(2) into Phi(2) + 144.
             - A Change of the Sense Transforms Phi(2) into 180 - Phi(2).


Pseudorotation Parameters P and Tau(M), (Rao, Westhof & Sundaralingam, Acta Cryst (1981), A37, 421-425)
----------------------------------------------------------------------------------------------------------------------------------
P =   354.5(1) Degree, Tau(M) =    35.9(1) Deg. for Reference Bond C(31) --> C(41)  [add 144 Deg. to P for each shift to next Bond]

Note: DELTA [Defined in Altona,C,Geise,H.J.,Romers,C.(1968). Tetrahedron, 24, 13-32] = 2 * P

Nearest Furanose Pucker Descriptor - (see W. Saenger, Principles of Nucleic Acid Structure, 1983, pp19
----------------------------------------------------------------------------------------------------------------------------------
Descriptor: T(wisted)  C(31) -exo , C(41) -endo     Absolute Configuration: D


Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

           Coefficients of Primitive and Normalised Forms
           M      Primitive  Coefficient Angular Value
           -----------------------------------------
CosForm    2        0.096        0.269        14.0
SinForm             0.260        0.731        15.0
                              Analysis of Ring Substituents
                              =============================
      Bond             Distance     Angle with C&P Plane Normal
-------------------------------------------------------------
C(21)   - O(1)       1.4286(17)           17.78(9)  Ax
C(21)   - C(11)      1.5241(13)           53.99(7)  Bi
```

C(31)	- O(31)	1.4031(18)	67.67(9)	Eq
C(41)	- O(41)	1.4190(16)	59.66(8)	Bi

C(51)	- C(61)	1.5135(15)	52.92(8)	Bi
C(31)	- H(31)	1.102(3)	5.96(16)	Ax
C(41)	- H(41)	1.097(3)	10.05(17)	Ax
C(51)	- H(51)	1.103(3)	19.55(16)	Ax

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  6-Membered Ring ( 2)   O(5)   -->   C(1)   -->   C(2)   -->   C(3)   -->   C(4)   -->   C(5)   -->
-------------------------------------------------------------------------------------------------------------------------
Dev. (Ang)             0.1976(13)   -0.2107(9)   0.2394(12)  -0.2550(12)   0.2418(12)  -0.2131(12)
Cs(I)-Asym-Par (Deg)      0.21(9)      0.95(9)      1.00(9)      0.21(9)      0.95(9)      1.00(9)
C2(I)-Asym-Par (Deg)    110.75(9)    110.74(9)    110.74(9)    110.75(9)    110.74(9)    110.74(9)
Ring Bond Angle(Deg)    115.96(9)    110.84(7)    111.02(7)    108.13(9)   110.81(10)    110.66(9)

Tors(I-J) (Deg)              -54.91(12)    54.99(11)   -56.03(11)    56.27(11)   -54.87(12)    55.16(12)
Cs(I-J)-Asym-Par   (Deg)    110.53(12)   111.19(12)   110.52(12)   110.53(12)   111.19(12)   110.52(12)
C2(I-J)-Asym-Par   (Deg)      0.83(12)     1.12(12)     0.91(11)     0.83(12)     1.12(12)     0.91(11)
Ring Bond Distance (Ang)    1.4108(14)   1.5346(13)   1.5198(18)   1.5257(15)   1.5258(17)   1.4386(19)

Weighted Average Ring Bond Distance = 1.4937(  6,227) Ang.  -  NOTE: 1st esd. Internal, 2nd esd External
Weighted Average Abs. Torsion Angl. =  55.41(  5, 26) Deg.           see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234

Cremer & Pople Puckering Parameters  [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]
-------------------------------------------------------------------------------------------------------------------------
Q(2)  =       0.050(1) Ang.,  Phi(2) =     182.8(13) Deg
Q(3)  =       0.554(1) Ang.

Puckering Amplitude (Q) =    0.556(1) Ang, Theta =       5.1(1) Deg,  Phi =    182.8(13) Deg


*** NOTE *** - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
             - A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
             - A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.


Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

           Coefficients of Primitive and Normalised Forms
           M      Primitive  Coefficient Angular Value
           -------------------------------------------
CosForm    2        0.045        0.075        12.0
SinForm             0.005        0.008        14.0
           3                     0.917         1.0

:: Note: This is Very Similar to a C-Form
                               Analysis of Ring Substituents
                               =============================
      Bond             Distance     Angle with C&P Plane Normal
---------------------------------------------------------------
C(1)    - O(1)       1.4216(13)           7.03(6)  Ax
C(2)    - O(2)       1.4247(16)          70.73(7)  Eq
C(3)    - O(3)         1.424(2)          69.04(9)  Eq
C(4)    - O(4)         1.410(2)          69.01(9)  Eq
C(5)    - C(6)       1.5228(15)          65.91(7)  Eq

C(1)    - H(1)         1.102(3)         62.75(16)  Eq
```

C(2)	- H(2)	1.106(2)	0.61(11)	Ax
C(3)	- H(3)	1.098(2)	1.23(11)	Ax
C(4)	- H(4)	1.102(2)	1.98(11)	Ax
C(5)	- H(5)	1.104(2)	4.85(11)	Ax

Analysis of Short Intra- and Inter-molecular Contacts , d(I-J) < R(I) + R(J) + Tolr, With Tolr = 0.2 Ang. (X - I...J) > 100. Deg.

Contact Radii :	C	H	O
(Angstrom)	1.70	1.20	1.52

Default Contact Radii are those given by A.Bondi, J.Phys.Chem. (1964),68,441. (or Coval. Rad. + 0.8 Ang. when not given)

* WARNING * : no Far-Reaching Conclusions should be drawn based on the Default Radii Assigned to Metals

Short "INTRA" Distances between two Atoms that are Separated by less than 4 Bonds are NOT Listed (Except for Potential D/A Contacts)

At(I)[1555.01]		At(J)	[ARU(J)]	D(I-J)	Sumrad	Del	Type	X(I)	Y(I)	Z(I)	X(J)	Y(J)	Z(J)	X	X - I...J
O(1)	....	O(2)	[ ]	2.8017(16)<<	3.04	-0.24	Intra	0.1714	0.3463	0.3916	0.2295	0.4355	0.7477	C(21)	112.11(7)
O(1)	....	O(11)	[ ]	2.7715(17)<<	3.04	-0.27	Intra	0.1714	0.3463	0.3916	0.0302	0.2355	0.6212	C(1)	108.55(7)
O(1)	....	O(31)	[ ]	2.7435(16)<<	3.04	-0.30	Intra	0.1714	0.3463	0.3916	-0.0737	0.3178	0.2045	C(1)	178.23(8)
O(1)	....	H(3)	[ ]	2.702(3) <	2.72	-0.02	Intra	0.1714	0.3463	0.3916	0.1871	0.6448	0.4897	C(21)	158.98(9)
O(1)	....	H(5)	[ ]	2.673(3) <	2.72	-0.05	Intra	0.1714	0.3463	0.3916	0.2638	0.5613	0.2093	C(21)	139.15(8)
O(1)	....	H(41)	[ ]	2.910(3)	2.72	0.19	Intra	0.1714	0.3463	0.3916	0.0984	0.2772	0.0155	C(1)	122.73(8)
O(1)	....	H(101)	[ ]	2.437(3)<<	2.72	-0.28	Intra	0.1714	0.3463	0.3916	0.0845	0.3247	0.6542		
O(1)	....	H(301)	[ ]	2.506(2)<<	2.72	-0.21	Intra	0.1714	0.3463	0.3916	-0.0310	0.4089	0.1761	C(1)	159.55(10)
O(2)	....	O(1)	[ ]	2.8017(16)<<	3.04	-0.24	Intra	0.2295	0.4355	0.7477	0.1714	0.3463	0.3916	H(23)	125.8(2)
O(2)	....	O(3)	[ ]	2.893(2) <	3.04	-0.15	Intra	0.2295	0.4355	0.7477	0.3080	0.7477	0.7028	H(23)	121.7(2)
O(2)	....	O(11)	[ ]	2.781(2)<<	3.04	-0.26	Intra	0.2295	0.4355	0.7477	0.0302	0.2355	0.6212	C(2)	118.98(9)
O(2)	....	O(61)	[1556.01]	2.855(2) <	3.04	-0.18		0.2295	0.4355	0.7477	0.3264	0.2380	1.0403	C(2)	117.21(9)
O(2)	....	C(11)	[ ]	3.231(2)	3.22	0.01	Intra	0.2295	0.4355	0.7477	0.1030	0.1311	0.5438		
O(2)	....	H(33)	[ ]	2.877(4)	2.72	0.16	Intra	0.2295	0.4355	0.7477	0.2318	0.7660	0.7426	H(23)	124.9(2)
O(2)	....	H(101)	[ ]	1.851(3)<<	2.72	-0.87	Intra	0.2295	0.4355	0.7477	0.0845	0.3247	0.6542	C(2)	119.06(12)
														H(23)	103.0(2)
O(2)	....	H(31)	[2556.01]	2.406(3)<<	2.72	-0.31		0.2295	0.4355	0.7477	0.0495	0.5884	0.7710	C(2)	123.29(12)
														H(23)	120.2(2)
O(3)	....	O(2)	[ ]	2.893(2) <	3.04	-0.15	Intra	0.3080	0.7477	0.7028	0.2295	0.4355	0.7477		
O(3)	....	O(4)	[ ]	2.879(2) <	3.04	-0.16	Intra	0.3080	0.7477	0.7028	0.3488	0.8141	0.3563	H(33)	126.3(2)
O(3)	....	H(43)	[ ]	2.534(5) <	2.72	-0.19	Intra	0.3080	0.7477	0.7028	0.3407	0.8913	0.4325	H(33)	118.4(3)
O(3)	....	O(6)	[2656.01]	2.849(2) <	3.04	-0.19		0.3080	0.7477	0.7028	0.4186	1.0453	0.7138	C(3)	129.78(10)
														H(33)	103.2(2)
O(3)	....	O(31)	[2556.01]	2.8618(19) <	3.04	-0.18		0.3080	0.7477	0.7028	0.0737	0.8178	0.7955	C(3)	108.75(9)
O(3)	....	H(63)	[2656.01]	1.921(4)<<	2.72	-0.80		0.3080	0.7477	0.7028	0.3985	0.9383	0.7134	C(3)	128.19(15)
														H(33)	108.2(3)
O(4)	....	O(3)	[ ]	2.879(2) <	3.04	-0.16	Intra	0.3488	0.8141	0.3563	0.3080	0.7477	0.7028		
O(4)	....	O(21)	[1565.01]	2.838(2)<<	3.04	-0.20		0.3488	0.8141	0.3563	0.2121	1.0944	0.3157	C(4)	148.65(12)
O(4)	....	C(51)	[1565.01]	3.127(2) <	3.22	-0.09		0.3488	0.8141	0.3563	0.1763	1.0613	0.1286	C(4)	154.57(12)
O(4)	....	C(61)	[1565.01]	3.306(2)	3.22	0.09		0.3488	0.8141	0.3563	0.2893	1.0819	0.0467	C(4)	162.10(10)
O(4)	....	H(6)	[ ]	2.517(4)<<	2.72	-0.20	Intra	0.3488	0.8141	0.3563	0.4531	0.6873	0.1345	H(43)	152.8(4)
O(4)	....	H(51)	[1565.01]	2.780(3)	2.72	0.06		0.3488	0.8141	0.3563	0.1465	0.9401	0.1133	C(4)	135.15(13)
O(4)	....	H(611)	[1565.01]	2.558(4) <	2.72	-0.16		0.3488	0.8141	0.3563	0.3672	1.0119	0.1195	C(4)	153.53(14)
O(4)	....	H(63)	[2656.01]	2.910(4)	2.72	0.19		0.3488	0.8141	0.3563	0.3985	0.9383	0.7134		
O(5)	....	O(6)	[ ]	2.7559(19)<<	3.04	-0.28	Intra	0.3772	0.3988	0.3686	0.5814	0.5453	0.2862	C(1)	153.16(8)

O(5)	....	O(21)	[ ]	3.1741(19)		3.04	0.13	Intra	0.3772	0.3988	0.3686	0.2121	0.0944	0.3157	C(5)	134.06(8)
O(5)	....	O(61)	[ ]	2.8497(19)	<	3.04	-0.19	Intra	0.3772	0.3988	0.3686	0.3264	0.2380	0.0404	C(1)	115.07(8)
O(5)	....	H(63)	[ ]	2.675(4)	<	2.72	-0.05	Intra	0.3772	0.3988	0.3686	0.6015	0.4383	0.2866	C(1)	152.99(11)
O(5)	....	H(601)	[ ]	1.894(3)	<<	2.72	-0.83	Intra	0.3772	0.3988	0.3686	0.3477	0.2780	0.1603	C(1)	113.23(13)
															C(5)	101.06(12)
O(5)	....	C(4)	[2646.01]	3.4083(17)		3.22	0.19		0.3772	0.3988	0.3686	0.6260	0.1709	0.5580	C(5)	136.96(8)

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 O(5)     ....  H(4)   [  2646.01]    2.612(3) < 2.72 -0.11        0.3772 0.3988 0.3686   0.5283 0.1681 0.4782   C(5)       148.94(9)
 O(6)     ....  O(5)   [         ]  2.7559(19)<< 3.04 -0.28 Intra  0.5814 0.5453 0.2862   0.3772 0.3988 0.3686
 O(6)     ....  H(4)   [         ]    2.623(3) < 2.72 -0.10 Intra  0.5814 0.5453 0.2862   0.4717 0.6681 0.5218   H(63)      122.2(3)
 O(6)     ....  O(3)   [  2646.01]    2.849(2) < 3.04 -0.19        0.5814 0.5453 0.2862   0.6920 0.2477 0.2972   C(6)      120.06(11)
 O(6)     ....  C(1)   [  2656.01]  3.3469(18)   3.22  0.13        0.5814 0.5453 0.2862   0.7004 0.8579 0.5151   C(6)      111.93(10)
                                                                                                               H(63)      136.8(2)
 O(6)     ....  C(61)  [  2655.01]  3.2202(19)   3.22  0.00        0.5814 0.5453 0.2862   0.7107 0.5819-0.0467
 O(6)     ....  H(1)   [  2656.01]    2.268(3)<< 2.72 -0.45        0.5814 0.5453 0.2862   0.6653 0.7451 0.4612   C(6)      114.65(13)
                                                                                                               H(63)      133.2(3)
 O(6)     ....  H(12)  [  2656.01]    2.436(3)<< 2.72 -0.28        0.5814 0.5453 0.2862   0.8053 0.6091 0.3670   C(6)      151.25(14)
 O(6)     ....  H(43)  [  2646.01]    2.539(5) < 2.72 -0.18        0.5814 0.5453 0.2862   0.6593 0.3913 0.5675   C(6)      130.78(18)
 O(6)     ....  H(62)  [  2655.01]    2.505(4)<< 2.72 -0.21        0.5814 0.5453 0.2862   0.7349 0.5399 0.0887   C(6)      109.99(12)
 O(11)    ....  O(1)   [         ]  2.7715(17)<< 3.04 -0.27 Intra  0.0302 0.2355 0.6212   0.1714 0.3463 0.3916
 O(11)    ....  O(2)   [         ]    2.781(2)<< 3.04 -0.26 Intra  0.0302 0.2355 0.6212   0.2295 0.4355 0.7477
 O(11)    ....  O(41)  [  1556.01]  2.7157(18)<< 3.04 -0.32        0.0302 0.2355 0.6212  -0.0212 0.0973 0.9110   C(11)     107.66(10)
                                                                                                               H(101)    111.11(16)
 O(11)    ....  C(41)  [  1556.01]  3.3542(15)   3.22  0.13        0.0302 0.2355 0.6212   0.0648 0.1665 1.0548   C(11)      111.15(8)
 O(11)    ....  H(401) [  1556.01]    1.760(3)<< 2.72 -0.96        0.0302 0.2355 0.6212  -0.0167 0.1538 0.8039   C(11)     111.73(14)
                                                                                                               H(101)    112.20(19)
 O(11)    ....  H(3)   [  2546.01]    2.455(3)<< 2.72 -0.27        0.0302 0.2355 0.6212  -0.1871 0.1448 0.5103   C(11)     103.21(11)
                                                                                                               H(101)     145.8(2)
 O(11)    ....  H(11)  [  2556.01]    2.796(3)   2.72  0.08        0.0302 0.2355 0.6212  -0.0520 0.5224 0.4784   C(11)     124.16(11)
 O(21)    ....  O(4)   [  1545.01]    2.838(2)<< 3.04 -0.20        0.2121 0.0944 0.3157   0.3488-0.1859 0.3563   C(21)      149.41(9)
 O(21)    ....  O(5)   [         ]  3.1741(19)   3.04  0.13 Intra  0.2121 0.0944 0.3157   0.3772 0.3988 0.3686   C(51)      108.25(8)
 O(21)    ....  O(61)  [         ]  2.9765(18) < 3.04 -0.06 Intra  0.2121 0.0944 0.3157   0.3264 0.2380 0.0404   C(21)      111.96(8)
 O(21)    ....  H(1)   [         ]    2.336(3)<< 2.72 -0.38 Intra  0.2121 0.0944 0.3157   0.3347 0.2451 0.5388   C(51)     146.76(11)
 O(21)    ....  H(43)  [  1545.01]    2.310(5)<< 2.72 -0.41        0.2121 0.0944 0.3157   0.3407-0.1087 0.4325   C(21)     137.65(15)
                                                                                                               C(51)     104.12(14)
 O(21)    ....  H(601) [         ]    2.641(3) < 2.72 -0.08 Intra  0.2121 0.0944 0.3157   0.3477 0.2780 0.1603   C(21)     104.45(11)
 O(31)    ....  O(1)   [         ]  2.7435(16)<< 3.04 -0.30 Intra -0.0737 0.3178 0.2045   0.1714 0.3463 0.3916
 O(31)    ....  O(41)  [         ]  3.1265(19)   3.04  0.09 Intra -0.0737 0.3178 0.2045  -0.0212 0.0973-0.0890
 O(31)    ....  O(3)   [  2546.01]  2.8618(19) < 3.04 -0.18       -0.0737 0.3178 0.2045  -0.3080 0.2477 0.2972   C(31)      113.48(9)
                                                                                                               H(301)    136.85(18)
 O(31)    ....  O(41)  [  2555.01]    2.864(2) < 3.04 -0.18       -0.0737 0.3178 0.2045   0.0212 0.5973 0.0890   C(31)      115.02(8)
 O(31)    ....  C(11)  [  2556.01]  3.4108(18)   3.22  0.19       -0.0737 0.3178 0.2045  -0.1030 0.6311 0.4562   C(31)      137.31(8)
 O(31)    ....  C(51)  [  2555.01]  3.3361(17)   3.22  0.12       -0.0737 0.3178 0.2045  -0.1763 0.5613-0.1286   C(31)      129.90(8)
 O(31)    ....  H(11)  [  2556.01]    2.742(3)   2.72  0.02       -0.0737 0.3178 0.2045  -0.0520 0.5224 0.4784   C(31)     121.58(10)
 O(31)    ....  H(33)  [  2546.01]    1.907(4)<< 2.72 -0.81       -0.0737 0.3178 0.2045  -0.2318 0.2660 0.2574   C(31)     112.58(14)
                                                                                                               H(301)     137.9(2)
 O(31)    ....  H(51)  [  2555.01]    2.639(3) < 2.72 -0.08       -0.0737 0.3178 0.2045  -0.1465 0.4401-0.1133   C(31)     115.09(10)
 O(31)    ....  H(62)  [  2555.01]    2.834(4)   2.72  0.11       -0.0737 0.3178 0.2045  -0.2651 0.5399 0.0887   C(31)     163.97(11)
 O(41)    ....  O(11)  [  1554.01]  2.7157(18)<< 3.04 -0.32       -0.0212 0.0973-0.0890   0.0302 0.2355-0.3788   C(41)      103.98(9)
 O(41)    ....  O(31)  [         ]  3.1265(19)   3.04  0.09 Intra -0.0212 0.0973-0.0890  -0.0737 0.3178 0.2045   H(401)    111.29(19)
 O(41)    ....  O(31)  [  2545.01]    2.864(2) < 3.04 -0.18       -0.0212 0.0973-0.0890   0.0737-0.1822-0.2045   C(41)      112.76(9)
 O(41)    ....  H(5)   [  2545.01]    2.610(3) < 2.72 -0.11       -0.0212 0.0973-0.0890  -0.2638 0.0613-0.2093   C(41)     140.03(10)
 O(41)    ....  H(301) [  2545.01]    1.908(3)<< 2.72 -0.81       -0.0212 0.0973-0.0890   0.0310-0.0911-0.1761   C(41)     116.59(12)
 O(61)    ....  O(2)   [  1554.01]    2.855(2) < 3.04 -0.18        0.3264 0.2380 0.0404   0.2295 0.4355-0.2523   C(61)      123.10(9)
                                                                                                               H(601)     120.8(2)
 O(61)    ....  O(5)   [         ]  2.8497(19) < 3.04 -0.19 Intra  0.3264 0.2380 0.0404   0.3772 0.3988 0.3686   C(61)      115.99(9)
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O(61)	....	O(21)	[ ]	2.9765(18) <	3.04	-0.06	Intra	0.3264	0.2380	0.0404	0.2121	0.0944	0.3157		
O(61)	....	C(5)	[ ]	3.339(2)	3.22	0.12	Intra	0.3264	0.2380	0.0404	0.3593	0.5511	0.2953	C(61)	138.86(9)
O(61)	....	C(6)	[ ]	3.311(2)	3.22	0.09	Intra	0.3264	0.2380	0.0404	0.4575	0.5708	0.1846	C(61)	158.26(9)
O(61)	....	H(23)	[1554.01]	1.892(3)<<	2.72	-0.83		0.3264	0.2380	0.0404	0.2719	0.3724	-0.1534	C(61)	125.28(14)
														H(601)	120.3(3)
O(61)	....	H(41)	[ ]	2.465(3)<<	2.72	-0.26	Intra	0.3264	0.2380	0.0404	0.0984	0.2772	0.0155		
O(61)	....	H(61)	[ ]	2.508(4)<<	2.72	-0.21	Intra	0.3264	0.2380	0.0404	0.4372	0.4927	0.0719	C(61)	167.25(13)

C(1)	....	H(12)	[ ]	2.810(3) <	2.90	-0.09	Intra	0.2996	0.3579	0.4849	0.1947	0.1091	0.6330	O(5)	144.17(8)
														C(2)	100.04(8)
C(1)	....	H(101)	[ ]	2.940(3)	2.90	0.04	Intra	0.2996	0.3579	0.4849	0.0845	0.3247	0.6542	O(5)	163.48(8)
C(1)	....	H(601)	[ ]	2.773(3) <	2.90	-0.13	Intra	0.2996	0.3579	0.4849	0.3477	0.2780	0.1603	C(2)	148.94(9)
C(1)	....	O(6)	[2646.01]	3.3469(18)	3.22	0.13		0.2996	0.3579	0.4849	0.4186	0.0453	0.7138	O(1)	115.46(6)
														O(5)	109.23(7)
														C(2)	100.08(6)
C(1)	....	H(4)	[2646.01]	2.994(2)	2.90	0.09		0.2996	0.3579	0.4849	0.5283	0.1681	0.4782	O(1)	132.37(7)
														C(2)	116.41(7)
C(2)	....	H(101)	[ ]	2.832(3) <	2.90	-0.07	Intra	0.3125	0.4747	0.6360	0.0845	0.3247	0.6542	C(3)	110.26(8)
														H(2)	135.41(16)
C(3)	....	H(63)	[2656.01]	3.016(4)	2.90	0.12		0.2855	0.6367	0.5645	0.3985	0.9383	0.7134	C(2)	129.70(9)
														H(3)	114.28(17)
C(4)	....	O(5)	[2656.01]	3.4083(17)	3.22	0.19		0.3740	0.6709	0.4420	0.6228	0.8988	0.6314	C(3)	113.26(7)
														C(5)	131.33(7)
C(5)	....	O(61)	[ ]	3.339(2)	3.22	0.12	Intra	0.3593	0.5511	0.2953	0.3264	0.2380	0.0404	C(4)	168.36(8)
C(5)	....	H(601)	[ ]	2.589(4)<<	2.90	-0.31	Intra	0.3593	0.5511	0.2953	0.3477	0.2780	0.1603	C(4)	156.50(10)
C(6)	....	O(61)	[ ]	3.311(2)	3.22	0.09	Intra	0.4575	0.5708	0.1846	0.3264	0.2380	0.0404	O(6)	109.51(10)
														H(6)	135.80(18)
C(6)	....	H(601)	[ ]	2.803(4) <	2.90	-0.10	Intra	0.4575	0.5708	0.1846	0.3477	0.2780	0.1603	O(6)	103.40(12)
														H(6)	147.5(2)
C(11)	....	O(2)	[ ]	3.231(2)	3.22	0.01	Intra	0.1030	0.1311	0.5438	0.2295	0.4355	0.7477	H(11)	159.12(18)
C(11)	....	H(1)	[ ]	2.714(3) <	2.90	-0.19	Intra	0.1030	0.1311	0.5438	0.3347	0.2451	0.5388	O(11)	112.19(10)
														H(11)	139.03(19)
C(11)	....	H(401)	[1556.01]	2.642(3)<<	2.90	-0.26		0.1030	0.1311	0.5438	-0.0167	0.1538	0.8039	C(21)	148.56(10)
C(11)	....	O(31)	[2546.01]	3.4108(18)	3.22	0.19		0.1030	0.1311	0.5438	0.0737	-0.1822	0.7955	C(21)	147.47(8)
C(31)	....	H(33)	[2546.01]	2.768(3) <	2.90	-0.13		0.0072	0.1908	0.2148	-0.2318	0.2660	0.2574	C(21)	122.68(8)
														C(41)	134.15(9)
C(41)	....	O(11)	[1554.01]	3.3542(15)	3.22	0.13		0.0648	0.1665	0.0548	0.0302	0.2355	-0.3788	C(31)	144.84(7)
														C(51)	112.68(6)
C(41)	....	H(301)	[2545.01]	2.842(3) <	2.90	-0.06		0.0648	0.1665	0.0548	0.0310	-0.0911	-0.1761	C(31)	127.13(9)
														H(41)	121.46(14)
C(51)	....	O(4)	[1545.01]	3.127(2) <	3.22	-0.09		0.1763	0.0613	0.1286	0.3488	-0.1859	0.3563	C(41)	161.96(8)
C(51)	....	H(43)	[1545.01]	3.008(5)	2.90	0.11		0.1763	0.0613	0.1286	0.3407	-0.1087	0.4325	C(41)	150.73(12)
C(51)	....	O(31)	[2545.01]	3.3361(17)	3.22	0.12		0.1763	0.0613	0.1286	0.0737	-0.1822	-0.2045	O(21)	150.81(9)
C(51)	....	H(301)	[2545.01]	2.859(3) <	2.90	-0.04		0.1763	0.0613	0.1286	0.0310	-0.0911	-0.1761	O(21)	153.85(9)
C(61)	....	O(4)	[1545.01]	3.306(2)	3.22	0.09		0.2893	0.0819	0.0467	0.3488	-0.1859	0.3563	O(61)	133.50(8)
														H(62)	115.5(2)
C(61)	....	H(23)	[1554.01]	2.951(3)	2.90	0.05		0.2893	0.0819	0.0467	0.2719	0.3724	-0.1534	C(51)	111.12(10)
														H(611)	134.5(2)
C(61)	....	O(6)	[2645.01]	3.2202(19)	3.22	0.00		0.2893	0.0819	0.0467	0.4186	0.0453	-0.2862	C(51)	149.93(8)
H(1)	....	O(21)	[ ]	2.336(3)<<	2.72	-0.38	Intra	0.3347	0.2451	0.5388	0.2121	0.0944	0.3157		
H(1)	....	C(11)	[ ]	2.714(3) <	2.90	-0.19	Intra	0.3347	0.2451	0.5388	0.1030	0.1311	0.5438		
H(1)	....	H(12)	[ ]	2.179(4)<<	2.40	-0.22	Intra	0.3347	0.2451	0.5388	0.1947	0.1091	0.6330	C(1)	113.81(18)
H(1)	....	O(6)	[2646.01]	2.268(3)<<	2.72	-0.45		0.3347	0.2451	0.5388	0.4186	0.0453	0.7138	C(1)	165.81(19)
H(1)	....	H(4)	[2646.01]	2.353(3) <	2.40	-0.05		0.3347	0.2451	0.5388	0.5283	0.1681	0.4782	C(1)	115.27(17)
H(2)	....	H(4)	[ ]	2.454(3)	2.40	0.05	Intra	0.4116	0.4693	0.7117	0.4717	0.6681	0.5218		
H(2)	....	H(611)	[2656.01]	2.493(4)	2.40	0.09		0.4116	0.4693	0.7117	0.6328	0.5119	0.8805	C(2)	169.0(2)
H(3)	....	O(1)	[ ]	2.702(3) <	2.72	-0.02	Intra	0.1871	0.6448	0.4897	0.1714	0.3463	0.3916		

H(3)	....	O(11)	[2556.01]	2.455(3)	<<	2.72	-0.27		0.1871	0.6448	0.4897	-0.0302	0.7355	0.3788	C(3)	162.1(2)
H(3)	....	H(401)	[2555.01]	2.595(3)		2.40	0.19		0.1871	0.6448	0.4897	0.0167	0.6538	0.1961	C(3)	152.16(18)
H(4)	....	O(6)	[ ]	2.623(3)	<	2.72	-0.10	Intra	0.4717	0.6681	0.5218	0.5814	0.5453	0.2862		
H(4)	....	H(2)	[ ]	2.454(3)		2.40	0.05	Intra	0.4717	0.6681	0.5218	0.4116	0.4693	0.7117		
H(4)	....	O(5)	[2656.01]	2.612(3)	<	2.72	-0.11		0.4717	0.6681	0.5218	0.6228	0.8988	0.6314	C(4)	128.39(19)
H(4)	....	C(1)	[2656.01]	2.994(2)		2.90	0.09		0.4717	0.6681	0.5218	0.7004	0.8579	0.5151	C(4)	132.51(18)
H(4)	....	H(1)	[2656.01]	2.353(3)	<	2.40	-0.05		0.4717	0.6681	0.5218	0.6653	0.7451	0.4612	C(4)	132.23(18)

H(5)	....	O(1)	[ ]	2.673(3)	<	2.72	-0.05	Intra	0.2638	0.5613	0.2093	0.1714	0.3463	0.3916		
H(5)	....	O(41)	[2555.01]	2.610(3)	<	2.72	-0.11		0.2638	0.5613	0.2093	0.0212	0.5973	0.0890	C(5)	164.23(18)
H(6)	....	O(4)	[ ]	2.517(4)	<<	2.72	-0.20	Intra	0.4531	0.6873	0.1345	0.3488	0.8141	0.3563		
H(11)	....	H(31)	[ ]	2.362(4)	<	2.40	-0.04	Intra	0.0520	0.0224	0.5216	-0.0495	0.0884	0.2290		
H(11)	....	O(11)	[2546.01]	2.796(3)		2.72	0.08		0.0520	0.0224	0.5216	-0.0302	-0.2645	0.3788	C(11)	160.6(2)
H(11)	....	O(31)	[2546.01]	2.742(3)		2.72	0.02		0.0520	0.0224	0.5216	0.0737	-0.1822	0.7955	C(11)	119.3(2)
H(11)	....	H(101)	[2546.01]	2.473(4)		2.40	0.07		0.0520	0.0224	0.5216	-0.0845	-0.1753	0.3458	C(11)	155.7(2)
H(12)	....	C(1)	[ ]	2.810(3)	<	2.90	-0.09	Intra	0.1947	0.1091	0.6330	0.2996	0.3579	0.4849		
H(12)	....	H(1)	[ ]	2.179(4)	<<	2.40	-0.22	Intra	0.1947	0.1091	0.6330	0.3347	0.2451	0.5388	C(11)	107.3(2)
H(12)	....	H(62)	[1556.01]	2.207(4)	<	2.40	-0.19		0.1947	0.1091	0.6330	0.2651	0.0399	0.9113	C(11)	137.1(2)
H(12)	....	O(6)	[2646.01]	2.436(3)	<<	2.72	-0.28		0.1947	0.1091	0.6330	0.4186	0.0453	0.7138	C(11)	156.49(18)
H(23)	....	O(61)	[1556.01]	1.892(3)	<<	2.72	-0.83		0.2719	0.3724	0.8466	0.3264	0.2380	1.0403	O(2)	170.2(3)
H(23)	....	C(61)	[1556.01]	2.951(3)		2.90	0.05		0.2719	0.3724	0.8466	0.2893	0.0819	1.0467	O(2)	149.7(3)
H(23)	....	H(61)	[1556.01]	2.443(4)		2.40	0.04		0.2719	0.3724	0.8466	0.4372	0.4927	1.0719	O(2)	117.7(3)
H(23)	....	H(101)	[ ]	2.277(4)	<	2.40	-0.12	Intra	0.2719	0.3724	0.8466	0.0845	0.3247	0.6542		
H(23)	....	H(601)	[1556.01]	2.526(3)		2.40	0.13		0.2719	0.3724	0.8466	0.3477	0.2780	1.1603	O(2)	160.0(3)
H(31)	....	H(11)	[ ]	2.362(4)	<	2.40	-0.04	Intra	-0.0495	0.0884	0.2290	0.0520	0.0224	0.5216		
H(31)	....	O(2)	[2546.01]	2.406(3)	<<	2.72	-0.31		-0.0495	0.0884	0.2290	-0.2295	-0.0645	0.2523	C(31)	159.43(19)
H(31)	....	H(33)	[2546.01]	2.560(4)		2.40	0.16		-0.0495	0.0884	0.2290	-0.2318	0.2660	0.2574		
H(31)	....	H(101)	[2546.01]	2.528(4)		2.40	0.13		-0.0495	0.0884	0.2290	-0.0845	-0.1753	0.3458	C(31)	154.41(19)
H(33)	....	O(2)	[ ]	2.877(4)		2.72	0.16	Intra	0.2318	0.7660	0.7426	0.2295	0.4355	0.7477		
H(33)	....	O(31)	[2556.01]	1.907(4)	<<	2.72	-0.81		0.2318	0.7660	0.7426	0.0737	0.8178	0.7955	O(3)	172.8(3)
H(33)	....	C(31)	[2556.01]	2.768(3)	<	2.90	-0.13		0.2318	0.7660	0.7426	-0.0072	0.6908	0.7851	O(3)	154.0(3)
H(33)	....	H(31)	[2556.01]	2.560(4)		2.40	0.16		0.2318	0.7660	0.7426	0.0495	0.5884	0.7710	O(3)	131.8(3)
H(33)	....	H(63)	[2656.01]	2.401(5)		2.40	0.00		0.2318	0.7660	0.7426	0.3985	0.9383	0.7134		
H(41)	....	O(1)	[ ]	2.910(3)		2.72	0.19	Intra	0.0984	0.2772	0.0155	0.1714	0.3463	0.3916		
H(41)	....	O(61)	[ ]	2.465(3)	<<	2.72	-0.26	Intra	0.0984	0.2772	0.0155	0.3264	0.2380	0.0404	C(41)	104.35(16)
H(41)	....	H(301)	[ ]	2.372(3)	<	2.40	-0.03	Intra	0.0984	0.2772	0.0155	-0.0310	0.4089	0.1761		
H(43)	....	O(3)	[ ]	2.534(5)	<	2.72	-0.19	Intra	0.3407	0.8913	0.4325	0.3080	0.7477	0.7028	O(4)	103.0(3)
H(43)	....	O(21)	[1565.01]	2.310(5)	<<	2.72	-0.41		0.3407	0.8913	0.4325	0.2121	1.0944	0.3157	O(4)	116.6(4)
H(43)	....	C(51)	[1565.01]	3.008(5)		2.90	0.11		0.3407	0.8913	0.4325	0.1763	1.0613	0.1286		
H(43)	....	O(6)	[2656.01]	2.539(5)	<	2.72	-0.18		0.3407	0.8913	0.4325	0.4186	1.0453	0.7138	O(4)	152.1(5)
H(43)	....	H(63)	[2656.01]	2.168(6)	<<	2.40	-0.23		0.3407	0.8913	0.4325	0.3985	0.9383	0.7134	O(4)	137.9(4)
H(51)	....	O(4)	[1545.01]	2.780(3)		2.72	0.06		0.1465	-0.0599	0.1133	0.3488	-0.1859	0.3563		
H(51)	....	O(31)	[2545.01]	2.639(3)	<	2.72	-0.08		0.1465	-0.0599	0.1133	0.0737	-0.1822	-0.2045	C(51)	120.42(16)
H(51)	....	H(301)	[2545.01]	2.330(3)	<	2.40	-0.07		0.1465	-0.0599	0.1133	0.0310	-0.0911	-0.1761	C(51)	107.31(17)
H(61)	....	O(61)	[ ]	2.508(4)	<<	2.72	-0.21	Intra	0.4372	0.4927	0.0719	0.3264	0.2380	0.0404	C(6)	129.5(2)
H(61)	....	H(23)	[1554.01]	2.443(4)		2.40	0.04		0.4372	0.4927	0.0719	0.2719	0.3724	-0.1534	C(6)	145.6(3)
H(61)	....	H(601)	[ ]	2.282(5)	<	2.40	-0.12	Intra	0.4372	0.4927	0.0719	0.3477	0.2780	0.1603	C(6)	107.1(2)
H(62)	....	H(12)	[1554.01]	2.207(4)	<	2.40	-0.19		0.2651	0.0399	-0.0887	0.1947	0.1091	-0.3670	C(61)	144.0(3)
H(62)	....	O(6)	[2645.01]	2.505(4)	<<	2.72	-0.21		0.2651	0.0399	-0.0887	0.4186	0.0453	-0.2862	C(61)	122.3(2)
H(62)	....	O(31)	[2545.01]	2.834(4)		2.72	0.11		0.2651	0.0399	-0.0887	0.0737	-0.1822	-0.2045	C(61)	122.5(2)
H(62)	....	H(63)	[2645.01]	2.497(5)		2.40	0.10		0.2651	0.0399	-0.0887	0.3985	-0.0617	-0.2866	C(61)	131.7(3)
H(63)	....	O(5)	[ ]	2.675(4)	<	2.72	-0.05	Intra	0.6015	0.4383	0.2866	0.3772	0.3988	0.3686		
H(63)	....	O(3)	[2646.01]	1.921(4)	<<	2.72	-0.80		0.6015	0.4383	0.2866	0.6920	0.2477	0.2972	O(6)	162.8(3)
H(63)	....	O(4)	[2646.01]	2.910(4)		2.72	0.19		0.6015	0.4383	0.2866	0.6512	0.3141	0.6437	O(6)	111.0(3)
H(63)	....	C(3)	[2646.01]	3.016(4)		2.90	0.12		0.6015	0.4383	0.2866	0.7146	0.1367	0.4355	O(6)	157.2(3)
H(63)	....	H(33)	[2646.01]	2.401(5)		2.40	0.00		0.6015	0.4383	0.2866	0.7682	0.2660	0.2574	O(6)	141.6(3)
H(63)	....	H(43)	[2646.01]	2.168(6)	<<	2.40	-0.23		0.6015	0.4383	0.2866	0.6593	0.3913	0.5675	O(6)	101.6(3)

H(63)	....	H(62)	[2655.01]	2.497(5)	2.40	0.10		0.6015	0.4383	0.2866	0.7349	0.5399	0.0887		
H(101)	....	O(1)	[ ]	2.437(3)<<	2.72	-0.28	Intra	0.0845	0.3247	0.6542	0.1714	0.3463	0.3916		
H(101)	....	O(2)	[ ]	1.851(3)<<	2.72	-0.87	Intra	0.0845	0.3247	0.6542	0.2295	0.4355	0.7477	O(11)	158.5(3)
H(101)	....	C(1)	[ ]	2.940(3)	2.90	0.04	Intra	0.0845	0.3247	0.6542	0.2996	0.3579	0.4849	O(11)	117.1(2)
H(101)	....	C(2)	[ ]	2.832(3) <	2.90	-0.07	Intra	0.0845	0.3247	0.6542	0.3125	0.4747	0.6360	O(11)	147.1(2)
H(101)	....	H(23)	[ ]	2.277(4) <	2.40	-0.12	Intra	0.0845	0.3247	0.6542	0.2719	0.3724	0.8466	O(11)	135.9(2)
H(101)	....	H(401)	[1556.01]	2.311(4) <	2.40	-0.09		0.0845	0.3247	0.6542	-0.0167	0.1538	0.8039		

```
==========================================================================================================================
 H(101)  ....  H(11)  [  2556.01]     2.473(4)   2.40  0.07        0.0845 0.3247 0.6542  -0.0520 0.5224 0.4784
 H(101)  ....  H(31)  [  2556.01]     2.528(4)   2.40  0.13        0.0845 0.3247 0.6542   0.0495 0.5884 0.7710   O(11)      133.4(3)
 H(301)  ....  O(1)   [          ]    2.506(2)<< 2.72 -0.21 Intra -0.0310 0.4089 0.1761   0.1714 0.3463 0.3916
 H(301)  ....  H(41)  [          ]    2.372(3) < 2.40 -0.03 Intra -0.0310 0.4089 0.1761   0.0984 0.2772 0.0155
 H(301)  ....  O(41)  [  2555.01]     1.908(3)<< 2.72 -0.81       -0.0310 0.4089 0.1761   0.0212 0.5973 0.0890   O(31)      168.5(2)
 H(301)  ....  C(41)  [  2555.01]     2.842(3) < 2.90 -0.06       -0.0310 0.4089 0.1761  -0.0648 0.6665-0.0548   O(31)    142.07(19)
 H(301)  ....  C(51)  [  2555.01]     2.859(3) < 2.90 -0.04       -0.0310 0.4089 0.1761  -0.1763 0.5613-0.1286   O(31)    111.38(17)
 H(301)  ....  H(51)  [  2555.01]     2.330(3) < 2.40 -0.07       -0.0310 0.4089 0.1761  -0.1465 0.4401-0.1133
 H(301)  ....  H(401) [  2555.01]     2.191(4)<< 2.40 -0.21       -0.0310 0.4089 0.1761   0.0167 0.6538 0.1961   O(31)      153.9(2)
 H(401)  ....  O(11)  [  1554.01]     1.760(3)<< 2.72 -0.96       -0.0167 0.1538-0.1961   0.0302 0.2355-0.3788   O(41)      165.4(3)
 H(401)  ....  C(11)  [  1554.01]     2.642(3)<< 2.90 -0.26       -0.0167 0.1538-0.1961   0.1030 0.1311-0.4562   O(41)      137.7(2)
 H(401)  ....  H(101) [  1554.01]     2.311(4) < 2.40 -0.09       -0.0167 0.1538-0.1961   0.0845 0.3247-0.3458   O(41)      150.7(3)
 H(401)  ....  H(3)   [  2545.01]     2.595(3)   2.40  0.19       -0.0167 0.1538-0.1961  -0.1871 0.1448-0.4897   O(41)      124.7(2)
 H(401)  ....  H(301) [  2545.01]     2.191(4)<< 2.40 -0.21       -0.0167 0.1538-0.1961   0.0310-0.0911-0.1761
 H(601)  ....  O(5)   [          ]    1.894(3)<< 2.72 -0.83 Intra  0.3477 0.2780 0.1603   0.3772 0.3988 0.3686   O(61)      167.0(3)
 H(601)  ....  O(21)  [          ]    2.641(3) < 2.72 -0.08 Intra  0.3477 0.2780 0.1603   0.2121 0.0944 0.3157   O(61)      100.6(2)
 H(601)  ....  C(1)   [          ]    2.773(3) < 2.90 -0.13 Intra  0.3477 0.2780 0.1603   0.2996 0.3579 0.4849   O(61)      155.1(3)
 H(601)  ....  C(5)   [          ]    2.589(4)<< 2.90 -0.31 Intra  0.3477 0.2780 0.1603   0.3593 0.5511 0.2953   O(61)      134.1(3)
 H(601)  ....  C(6)   [          ]    2.803(4) < 2.90 -0.10 Intra  0.3477 0.2780 0.1603   0.4575 0.5708 0.1846   O(61)      113.4(2)
 H(601)  ....  H(23)  [  1554.01]     2.526(3)   2.40  0.13        0.3477 0.2780 0.1603   0.2719 0.3724-0.1534
 H(601)  ....  H(61)  [          ]    2.282(5) < 2.40 -0.12 Intra  0.3477 0.2780 0.1603   0.4372 0.4927 0.0719
 H(611)  ....  O(4)   [  1545.01]     2.558(4) < 2.72 -0.16        0.3672 0.0119 0.1195   0.3488-0.1859 0.3563   C(61)      124.8(2)
 H(611)  ....  H(2)   [  2646.01]     2.493(4)   2.40  0.09        0.3672 0.0119 0.1195   0.5884-0.0307 0.2883   C(61)      154.0(3)
```

```
Summary of Shortest Inter Contacts with d(I-J) <  R(I) + R(J) +  0.2 of Residue #  1 to Neighbouring ARU'S
==========================================================================================================================

  Nr       ARU    Nr.Cont.   d(min)    Del  XHn X      - At(I)       At(J)  - Y    YHn  Note  Partaking ARU's in Close Contact Resd.
--------------------------------------------------------------------------------------------------------------------------
   1 [  1556.01]      11     1.7600  -0.96    2 C(11)  - O(11)  ...  H(401) -O(41)   1   <<   1556.01
   2 [  2556.01]      11     1.9070  -0.81    1 O(3)   - H(33)  ...  O(31)  -C(31)   1   <<   2556.01
   3 [  2656.01]      15     1.9210  -0.80    1 C(3)   - O(3)   ...  H(63)  -O(6)    1   <<   2656.01
   4 [  1565.01]       7     2.3100  -0.41    1 O(4)   - H(43)  ...  O(21)  -C(21)   0   <<   1565.01
   5 [  2646.01]      15     1.9210  -0.80    1 O(6)   - H(63)  ...  O(3)   -C(3)    1   <<   2646.01
   6 [  2655.01]       3     2.4970   0.10    1 O(6)   - H(63)  ...  H(62)  -C(61)   2        2655.01
   7 [  2546.01]      11     1.9070  -0.81    1 C(31)  - O(31)  ...  H(33)  -O(3)    1   <<   2546.01
   8 [  1545.01]       7     2.3100  -0.41    0 C(21)  - O(21)  ...  H(43)  -O(4)    1   <<   1545.01
   9 [  2555.01]      11     1.9080  -0.81    1 O(31)  - H(301) ...  O(41)  -C(41)   1   <<   2555.01
  10 [  1554.01]      11     1.7600  -0.96    1 O(41)  - H(401) ...  O(11)  -C(11)   2   <<   1554.01
  11 [  2545.01]      11     1.9080  -0.81    1 C(41)  - O(41)  ...  H(301) -O(31)   1   <<   2545.01
  12 [  2645.01]       3     2.4970   0.10    2 C(61)  - H(62)  ...  H(63)  -O(6)    1        2645.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
           NR.CONT. = Number of short contacts from current ARU to surrounding ARU's (from list above).

                                          Asymmetric Residue Unit (= ARU) Code List
                                          =========================================
```

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
[1556.01]	= x,y,1+z	= [1	0	0	1	1]	0.233	0.366	1.345
[2556.01]	= -x,1/2+y,1-z	= [2	0	0	1	1]	-0.233	0.866	0.655

[2656.01]	= 1-x,1/2+y,1-z	= [	2	1	0	1	1]	0.767	0.866	0.655
[1565.01]	= x,1+y,z	= [	1	0	1	0	1]	0.233	1.366	0.345
[2646.01]	= 1-x,-1/2+y,1-z	= [	2	1	-1	1	1]	0.767	-0.134	0.655
[2655.01]	= 1-x,1/2+y,-z	= [	2	1	0	0	1]	0.767	0.866	-0.345
[2546.01]	= -x,-1/2+y,1-z	= [	2	0	-1	1	1]	-0.233	-0.134	0.655
[1545.01]	= x,-1+y,z	= [	1	0	-1	0	1]	0.233	-0.634	0.345
[2555.01]	= -x,1/2+y,-z	= [	2	0	0	0	1]	-0.233	0.866	-0.345
[1554.01]	= x,y,-1+z	= [	1	0	0	-1	1]	0.233	0.366	-0.655
[2545.01]	= -x,-1/2+y,-z	= [	2	0	-1	0	1]	-0.233	-0.134	-0.345
[2645.01]	= 1-x,-1/2+y,-z	= [	2	1	-1	0	1]	0.767	-0.134	-0.345

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
Ires - Residue Number.
TX, TY, TZ - Unit Cell Translations.

```
==================================================================================================================================
Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks   (Minor Disorder Excluded)
==================================================================================================================================

Contact-Nr Atom I[   ARU   ]      Atom J[   ARU   ]    d(I-J)   Del
----------------------------------------------------------------------------------------------------------------------------------
   1       O(4)  [  1555.01] ...  O(21) [  1565.01] =  2.838  -0.20
   2       O(11) [  1555.01] ...  O(41) [  1556.01] =  2.716  -0.32
   3       O(21) [  1555.01] ...  O(4)  [  1545.01] =  2.838  -0.20
   4       O(41) [  1555.01] ...  O(11) [  1554.01] =  2.716  -0.32

                                                         ==============
********************************************************  CLUSTER  =  1***********************************************************
                                                         ==============

(N:M)  :  ARU   --    Connected  with (N) Interactions to/from (M) ARU(S).    T = Translated Molecule (Infinite chain etc.)
----------------------------------------------------------------------------------------------------------------------------------
 4  4  1555.01  --   1565.01T  1556.01T  1545.01T  1554.01T

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Two-Dimensional Network :: Base Vectors: #1 = [  0  1  0],  #2 = [  0  0  1],  - Plane: (  1  0  0)

                                                         ==============
********************************************************  CLUSTER  =  2***********************************************************
                                                         ==============

(N:M)  :  ARU   --    Connected  with (N) Interactions to/from (M) ARU(S).    T = Translated Molecule (Infinite chain etc.)
----------------------------------------------------------------------------------------------------------------------------------
 4  4  2555.01  --   2565.01T  2554.01T  2545.01T  2556.01T

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Two-Dimensional Network :: Base Vectors: #1 = [  0  1  0],  #2 = [  0  0  1],  - Plane: (  1  0  0)
```

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

Nr	Typ	Res	Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)
1		1	O(2) -- H(23) .. O(61)	[1556.01]	0.972(3)	1.892(3)	2.855(2)	170.2(3)				
2		1	O(3) -- H(33) .. O(31)	[2556.01]	0.960(4)	1.907(4)	2.8618(19)	172.8(3)				
3	Intra	1	O(4) -- H(43) .. O(3)	[ ]	0.912(4)	2.534(5)	2.879(2)	103.0(3)				
4		1	O(4) -- H(43) .. O(21)	[1565.01]	0.912(4)	2.310(5)	2.838(2)	116.6(4)'	121.2(3)'		340.8(6)	
5		1	O(4) -- H(43) .. O(6)	[2656.01]	0.912(4)	2.539(5)	3.373(2)	152.1(5)"	68.32(13)"	89.35(14)	323.4(6)	358.1(7)
6		1	O(6) -- H(63) .. O(3)	[2646.01]	0.956(4)	1.921(4)	2.849(2)	162.8(3)				
7	Intra	1	O(11) -- H(101).. O(2)	[ ]	0.974(3)	1.851(3)	2.781(2)	158.5(3)				
8		1	O(31) -- H(301).. O(41)	[2555.01]	0.969(3)	1.908(3)	2.864(2)	168.5(2)				
9		1	O(41) -- H(401).. O(11)	[1554.01]	0.976(3)	1.760(3)	2.7157(18)	165.4(3)				
10	Intra	1	O(61) -- H(601).. O(5)	[ ]	0.972(3)	1.894(3)	2.8497(19)	167.0(3)				
11		1	C(1) -- H(1) .. O(6)	[2646.01]	1.102(3)	2.268(3)	3.3469(18)	165.81(19)				
12		1	C(3) -- H(3) .. O(11)	[2556.01]	1.098(2)	2.455(3)	3.5153(17)	162.1(2)				
13		1	C(11) -- H(12) .. O(6)	[2646.01]	1.095(3)	2.436(3)	3.4673(18)	156.49(18)				
14		1	C(31) -- H(31) .. O(2)	[2546.01]	1.102(3)	2.406(3)	3.4597(18)	159.43(19)				
15	Intra	1	C(41) -- H(41) .. O(61)	[ ]	1.097(3)	2.465(3)	2.9363(18)	104.35(16)				
16	Intra	1	C(6) -- H(61) .. O(61)	[ ]	1.090(4)	2.508(4)	3.311(2)	129.5(2)				
17		1	C(61) -- H(62) .. O(6)	[2645.01]	1.087(3)	2.505(4)	3.2202(19)	122.3(2)				
18		1	C(61) -- H(611).. O(4)	[1545.01]	1.092(4)	2.558(4)	3.306(2)	124.8(2)				

Translation of ARU-code to Equivalent Position Code

```
   [  1556.00 ]  = x,y,1+z
   [  2556.00 ]  = -x,1/2+y,1-z
   [  2656.00 ]  = 1-x,1/2+y,1-z
   [  1565.00 ]  = x,1+y,z
   [  2646.00 ]  = 1-x,-1/2+y,1-z
   [  2546.00 ]  = -x,-1/2+y,1-z
   [  1545.00 ]  = x,-1+y,z
   [  2555.00 ]  = -x,1/2+y,-z
   [  1554.00 ]  = x,y,-1+z
   [  2645.00 ]  = 1-x,-1/2+y,-z
```

For C--H...Acceptor Interactions See: Th. Steiner, Cryst. Rev, (1996), 6, 1-57

H-Bond classification [G.A.Jeffrey, H.Maluszynska & J.Mitra., Int.J.Biol.Macromol.(1985),7,336-348]

```
2-Centre   (linear)     D-H...X most prob. angle 160 deg  - also: G.A.Jeffrey & W.Saenger, Hydrogen Bonding in Biological Structures
3-Centre (bifurcated)   SUM of 3 angl. about H = 360 deg                    Springer-Verlag, Berlin, 1991, pp 20.
4-Centre (trifurcated)
```

Analysis of Potential Donor/Acceptor Atoms -- (Major Disorder Form Only)

===

At.Nr	D/A	#Cov.Bonds	# H	#D-H..A	#A..H	#A..H-C	Sum(A-H)	Sum(A-X)
1	O(1)	2	-	0	0	0	0	2
2	O(2)	2	1 H	1	1	1	3	4
3	O(3)	2	1 H	1	2	0	3	4

4	O(4)	2	1 H	3	0	1	4	5
5	O(5)	2	-	0	1	0	1	3
6	O(6)	2	1 H	1	1	3	5	6
7	O(11)	2	1 H	1	1	1	3	4
8	O(21)	2	-	0	1	0	1	3
9	O(31)	2	1 H	1	1	0	2	3
10	O(41)	2	1 H	1	1	0	2	3
11	O(61)	2	1 H	1	1	2	4	5

Analysis of Hydrogen Bonded Molecular Aggregates (See also Acta Cryst. B36, 1980, 2113 - 2115) -- (Major Disorder Component Only)

Coordinates of Donor and Acceptor Atoms — Coordinates of D/A-Bonded Atom(s)

D/A I	[ARU]	X	Y	Z	--	D/A J	[ARU]	X	Y	Z	Atom K	X	Y	Z	I..J--K Angle
O(2)	[1555.01],	0.2295	0.4355	0.7477	>>	O(61)	[1556.01],	0.3264	0.2380	1.0403	C(61)	0.2893	0.0819	1.0467	123.10(10)
											H(601)	0.3477	0.2780	1.1603	120.81(16)
O(61)	[1555.01],	0.3264	0.2380	0.0404	<<	O(2)	[1554.01],	0.2295	0.4355	-0.2523	C(2)	0.3125	0.4747	-0.3640	117.21(10)
											H(23)	0.2719	0.3724	-0.1534	6.45(11)
O(3)	[1555.01],	0.3080	0.7477	0.7028	>>	O(31)	[2556.01],	0.0737	0.8178	0.7955	C(31)	-0.0072	0.6908	0.7851	113.48(11)
											H(301)	0.0310	0.9089	0.8239	136.85(15)
O(31)	[1555.01],	-0.0737	0.3178	0.2045	<<	O(3)	[2546.01],	-0.3080	0.2477	0.2972	C(3)	-0.2855	0.1367	0.4355	108.75(10)
											H(33)	-0.2318	0.2660	0.2574	4.82(11)
O(4)	[1555.01],	0.3488	0.8141	0.3563	>>	O(3)	[1555.01],	0.3080	0.7477	0.7028	C(3)	0.2855	0.6367	0.5645	57.92(9)
											H(33)	0.2318	0.7660	0.7426	126.26(14)
O(3)	[1555.01],	0.3080	0.7477	0.7028	<<	O(4)	[1555.01],	0.3488	0.8141	0.3563	C(4)	0.3740	0.6709	0.4420	55.72(8)
											H(43)	0.3407	0.8913	0.4325	59.03(13)
O(4)	[1555.01],	0.3488	0.8141	0.3563	>>	O(21)	[1565.01],	0.2121	1.0944	0.3157	C(21)	0.1245	1.1926	0.3690	149.41(12)
											C(51)	0.1763	1.0613	0.1286	87.47(10)
O(21)	[1555.01],	0.2121	0.0944	0.3157	<<	O(4)	[1545.01],	0.3488	-0.1859	0.3563	C(4)	0.3740	-0.3291	0.4420	148.65(10)
											H(43)	0.3407	-0.1087	0.4325	46.70(12)
O(4)	[1555.01],	0.3488	0.8141	0.3563	>>	O(6)	[2656.01],	0.4186	1.0453	0.7138	C(6)	0.5425	1.0708	0.8155	124.18(11)
											H(63)	0.3985	0.9383	0.7134	53.64(11)
O(6)	[1555.01],	0.5814	0.5453	0.2862	<<	O(4)	[2646.01],	0.6512	0.3141	0.6437	C(4)	0.6260	0.1709	0.5580	98.95(9)
											H(43)	0.6593	0.3913	0.5675	20.61(11)
O(6)	[1555.01],	0.5814	0.5453	0.2862	>>	O(3)	[2646.01],	0.6920	0.2477	0.2972	C(3)	0.7146	0.1367	0.4355	129.78(11)
											H(33)	0.7682	0.2660	0.2574	103.16(16)
O(3)	[1555.01],	0.3080	0.7477	0.7028	<<	O(6)	[2656.01],	0.4186	1.0453	0.7138	C(6)	0.5425	1.0708	0.8155	120.06(12)
											H(63)	0.3985	0.9383	0.7134	11.49(11)
O(11)	[1555.01],	0.0302	0.2355	0.6212	>>	O(2)	[1555.01],	0.2295	0.4355	0.7477	C(2)	0.3125	0.4747	0.6360	118.98(10)
											H(23)	0.2719	0.3724	0.8466	96.80(14)
O(2)	[1555.01],	0.2295	0.4355	0.7477	<<	O(11)	[1555.01],	0.0302	0.2355	0.6212	C(11)	0.1030	0.1311	0.5438	94.93(10)
											H(101)	0.0845	0.3247	0.6542	14.10(11)
O(31)	[1555.01],	-0.0737	0.3178	0.2045	>>	O(41)	[2555.01],	0.0212	0.5973	0.0890	C(41)	-0.0648	0.6665	-0.0548	112.76(11)
											H(401)	0.0167	0.6538	0.1961	94.09(14)
O(41)	[1555.01],	-0.0212	0.0973	-0.0890	<<	O(31)	[2545.01],	0.0737	-0.1822	-0.2045	C(31)	-0.0072	-0.3092	-0.2148	115.02(10)
											H(301)	0.0310	-0.0911	-0.1761	7.64(10)
O(41)	[1555.01],	-0.0212	0.0973	-0.0890	>>	O(11)	[1554.01],	0.0302	0.2355	-0.3788	C(11)	0.1030	0.1311	-0.4562	107.66(11)
											H(101)	0.0845	0.3247	-0.3458	111.11(13)
O(11)	[1555.01],	0.0302	0.2355	0.6212	<<	O(41)	[1556.01],	-0.0212	0.0973	0.9110	C(41)	0.0648	0.1665	1.0548	103.98(10)
											H(401)	-0.0167	0.1538	0.8039	9.37(10)
O(61)	[1555.01],	0.3264	0.2380	0.0404	>>	O(5)	[1555.01],	0.3772	0.3988	0.3686	C(1)	0.2996	0.3579	0.4849	115.07(11)
											C(5)	0.3593	0.5511	0.2953	96.72(9)
O(5)	[1555.01],	0.3772	0.3988	0.3686	<<	O(61)	[1555.01],	0.3264	0.2380	0.0404	C(61)	0.2893	0.0819	0.0467	115.99(10)
											H(601)	0.3477	0.2780	0.1603	8.59(12)

```
==============
****************************************************** AGGREGATE =  1***********************************************************
==============

(N:M)  :  ARU   --    Connected with N Hydrogen Bonds to/from M ARU(S).    T = Translated Molecule (Infinite chain etc.)
-----------------------------------------------------------------------------------------------------------------------------
14 10  1555.01  --   1556.01T  2556.01   1565.01T  2656.01T  2646.01T  2555.01T  1554.01T  2546.01T  1545.01T  2545.01T
14 10  2556.01  --   2555.01T  1565.01T  2566.01T  1465.01T  1455.01T  1566.01T  2557.01T  1555.01   2546.01T  1556.01T

:: Analysis of Polymeric Structure(s)

:: Resd # 0 - Infinite Three-Dimensional Framework :: Det = 1, Base Vectors:  #1 =[  0  0  1],  #2 =[  0  1  0],  #3 =[  1  0  0],

Search for ARU-Circuits (Max = 15) and Infinite ARU-Chains (Max =  4)
=============================================================================================================================


 15-Membered ARU-Circuit
  1555.01  1556.01  1557.01  1558.01  1568.01  1578.01  1588.01  2588.01  2587.01  2586.01  2585.01  1484.01  2575.01  2565.01
  2555.01  1555.01

 15-Membered ARU-Circuit
  1555.01  1556.01  1557.01  1558.01  1568.01  1578.01  1588.01  2588.01  2587.01  2586.01  2585.01  1484.01  2575.01  2565.01
  1565.01  1555.01

 15-Membered ARU-Circuit
  1555.01  1556.01  1557.01  1558.01  1568.01  1578.01  1588.01  2588.01  2587.01  2586.01  2585.01  1484.01  2575.01  1575.01
  1565.01  1555.01

  1-Membered Infinite ARU-Chain (Translation [  0  0  1])
  1555.01  1556.01
```

Analysis of the (Cooperative) Hydrogen Bond Network (i.e. (In)Finite O-H...O-H...O-H.. Chains and/or Rings (Max = 18 Membered))

** NetworK = 1 **

Code	Acc	Donor Atom		X	Y	Z	Acceptor Atom		X	Y	Z	up to BondCode(s) of Forward Link(s)
1.555		O(4)	[1555.01]	0.3488	0.8141	0.3563	O(3)	[1555.01]	0.3080	0.7477	0.7028	4.555
2.555		O(4)	[1555.01]	0.3488	0.8141	0.3563	O(21)	[1565.01]	0.2121	1.0944	0.3157	
3.555		O(4)	[1555.01]	0.3488	0.8141	0.3563	O(6)	[2656.01]	0.4186	1.0453	0.7138	5.555R
4.555	A	O(3)	[1555.01]	0.3080	0.7477	0.7028	O(31)	[2556.01]	0.0737	0.8178	0.7955	6.555
5.555	A	O(6)	[2656.01]	0.4186	1.0453	0.7138	O(3)	[1555.01]	0.3080	0.7477	0.7028	4.555
6.555	A	O(31)	[2556.01]	0.0737	0.8178	0.7955	O(41)	[1566.01]	-0.0212	1.0973	0.9110	7.555
7.555	A	O(41)	[1566.01]	-0.0212	1.0973	0.9110	O(11)	[1565.01]	0.0302	1.2355	0.6212	8.555
8.555	A	O(11)	[1565.01]	0.0302	1.2355	0.6212	O(2)	[1565.01]	0.2295	1.4355	0.7477	9.555
9.555	A	O(2)	[1565.01]	0.2295	1.4355	0.7477	O(61)	[1566.01]	0.3264	1.2380	1.0403	10.555
10.555	A	O(61)	[1566.01]	0.3264	1.2380	1.0403	O(5)	[1566.01]	0.3772	1.3988	1.3686	

Hydrogen Bonds are Coded as N.IJK Where N = Sequence Number of Hydrogen Bond (NOTE: New Hbond Numbering system)
I - 5 = Nr of Translation Units Along A-Axis
J - 5 = Nr of Translation Units Along B-Axis
K - 5 = Nr of Translation Units Along C-Axis

Ring Closure Links are Indicated with ’R’ and Infinite Chain Links With ’T’

Analysis of the Coordination Geometry

Distances are calculated from atom I of Unique Molecule Coordinate List to atom J in Asymmetric Residue Unit: ARU.

Phi = Azimuth angle(counter clockwise from XO in XO,YO-Plane), Mu = Angle between D and XO,YO-plane.

'To-Code' : '--' = Bonded atoms, '<<' = .LT. sum vdW-radii - 0.2, '.<' = .LT. sum vdW-radii, '..' = .GT. sum vdW-radii.

>>>> NOTICE >>>> : The Symmetry Code Character Added to the Atom Label Applies to the Current Coordination Sphere Only.
>>>>>>>>>>>>>>>> : Symmetry operations refer to the coordinates listed in the fractional coordinate table given above

The List May be Limited to the Shortest Distances.

3.6 Angstrom Coordination Sphere Around Atom I = O(1) [ARU = 1555.01]   0.17143 0.34630 0.39165   1.1816 3.0145 2.9614

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	1.4216(13)	--	C(1)	[=	]	Intra	4.70	29.72	0.29961	0.35792	0.48487	2.4120	3.1157	3.6663
2	1.4286(17)	--	C(21)	[=	]	Intra	-109.39	-6.90	0.12446	0.19262	0.36895	0.7108	1.6768	2.7897
3	2.3271(15)	<<	O(5)	[=	]	Intra	11.35	-4.29	0.37719	0.39878	0.36864	3.4568	3.4714	2.7874
4	2.3377(19)	<<	O(21)	[=	]	Intra	-75.35	-14.22	0.21205	0.09445	0.31572	1.7548	0.8222	2.3873
5	2.4088(15)	<<	C(31)	[=	]	Intra	-137.49	-33.71	0.00718	0.19075	0.21485	-0.2954	1.6605	1.6245
6	2.4183(17)	<<	C(11)	[=	]	Intra	-118.28	28.41	0.10301	0.13110	0.54380	0.1739	1.1412	4.1118
7	2.4273(15)	<<	C(2)	[=	]	Intra	45.26	49.57	0.31253	0.47474	0.63600	2.2897	4.1326	4.8090
8	2.7435(16)	<<	O(31)	[=	]	Intra	-173.93	-31.05	-0.07367	0.31776	0.20452	-1.1558	2.7661	1.5464
9	2.7715(17)	<<	O(11)	[=	]	Intra	-153.49	38.77	0.03017	0.23550	0.62119	-0.7519	2.0500	4.6970
10	2.8017(16)	<<	O(2)	[=	]	Intra	89.08	73.91	0.22954	0.43550	0.74766	1.1941	3.7910	5.6533
11	2.9296(16)	<<	C(5)	[=	]	Intra	38.92	-14.40	0.35925	0.55107	0.29529	3.3894	4.7971	2.2328
12	2.9966(17)	<<	C(3)	[=	]	Intra	69.64	25.85	0.28545	0.63673	0.56447	2.1199	5.5427	4.2681
13	3.0440(15)	.<	C(41)	[=	]	Intra	-110.11	-56.81	0.06478	0.16653	0.05476	0.6086	1.4496	0.4141
14	3.2201(17)	..	C(51)	[=	]	Intra	-78.37	-38.14	0.17635	0.06133	0.12864	1.6922	0.5339	0.9727
15	3.3517(18)	..	O(41)a	[-x,1/2+y,-z =	2555.01]		116.84	-43.05	0.02123	0.59734	0.08904	0.0759	5.1998	0.6733
16	3.5494(17)	..	C(4)	[=	]	Intra	53.21	6.15	0.37404	0.67095	0.44198	3.2951	5.8406	3.3420
17	2.078(3)	<<	H(1)	[=	]	Intra	-30.13	32.37	0.33470	0.24510	0.53880	2.6995	2.1336	4.0740
18	2.437(3)	<<	H(101)	[=	]	Intra	-172.35	54.55	0.08450	0.32470	0.65420	-0.2191	2.8265	4.9466
19	2.506(2)	<<	H(301)	[=	]	Intra	163.37	-40.56	-0.03100	0.40890	0.17610	-0.6428	3.5595	1.3315
20	2.673(3)	.<	H(5)	[=	]	Intra	54.80	-31.05	0.26380	0.56130	0.20930	2.5020	4.8861	1.5826
21	2.702(3)	.<	H(3)	[=	]	Intra	90.00	15.92	0.18710	0.64480	0.48970	1.1814	5.6130	3.7028
22	2.761(3)	..	H(12)	[=	]	Intra	-94.62	41.38	0.19470	0.10910	0.63300	1.0149	0.9497	4.7863
23	2.910(3)	..	H(41)	[=	]	Intra	-103.06	-77.75	0.09840	0.27720	0.01550	1.0420	2.4130	0.1172
24	2.963(3)	..	H(601)	[=	]	Intra	-14.39	-36.18	0.34770	0.27800	0.16030	3.4986	2.4200	1.2121
25	3.070(3)	..	H(11)b	[-x,1/2+y,1-z =	2556.01]		149.26	12.34	-0.05200	0.52240	0.47840	-1.3964	4.5475	3.6173
26	3.322(3)	..	H(31)	[=	]	Intra	-133.32	-21.73	-0.04950	0.08840	0.22900	-0.9357	0.7695	1.7315
27	3.339(3)	..	H(401)a	[-x,1/2+y,-z =	2555.01]		116.61	-26.28	0.01670	0.65380	0.19610	-0.1594	5.6913	1.4828
28	3.349(3)	..	H(2)	[=	]	Intra	27.55	46.27	0.41160	0.46930	0.71170	3.2344	4.0853	5.3814
29	3.352(3)	..	H(11)	[=	]	Intra	-118.38	17.05	0.05200	0.02240	0.52160	-0.3417	0.1950	3.9440
30	3.461(2)	..	H(23)	[=	]	Intra	37.07	83.75	0.27190	0.37240	0.84660	1.4823	3.2417	6.4014

Angles (Degrees) At1...V...At2 with Vertex V = O(1)

C(1)	C(21)	114.30(9)	C(1)	O(5)	34.60(5)	C(1)	O(21)	88.64(6)	C(1)	C(31)	147.77(8)
C(1)	C(11)	100.36(7)	C(1)	C(2)	36.36(5)	C(1)	O(31)	178.23(8)	C(1)	O(11)	108.55(7)
C(1)	O(2)	60.00(6)	C(1)	C(5)	55.09(5)	C(1)	C(3)	56.82(5)	C(1)	C(41)	127.91(7)
C(1)	C(51)	102.93(6)	C(1)	O(41)a	125.28(7)	C(1)	C(4)	51.30(5)	C(1)	H(1)	29.83(7)
C(1)	H(101)	95.68(9)	C(1)	H(301)	159.55(10)	C(1)	H(5)	77.20(7)	C(1)	H(3)	78.21(7)
C(1)	H(12)	77.16(7)	C(1)	H(41)	122.73(8)	C(1)	H(601)	68.30(7)	C(1)	H(11)b	125.82(9)
C(1)	H(31)	141.56(8)	C(1)	H(401)a	120.67(8)	C(1)	H(2)	24.29(6)	C(1)	H(11)	107.93(8)
C(1)	H(23)	55.06(7)	C(21)	O(5)	119.81(8)	C(21)	O(21)	34.21(5)	C(21)	C(31)	37.33(5)
C(21)	C(11)	36.33(5)	C(21)	C(2)	132.32(8)	C(21)	O(31)	64.69(6)	C(21)	O(11)	61.28(6)
C(21)	O(2)	112.11(7)	C(21)	C(5)	142.02(7)	C(21)	C(3)	161.02(7)	C(21)	C(41)	49.91(5)

C(21)	,	C(51)	41.98(5)	C(21)	,	O(41)a	114.82(7)	C(21)	,	C(4)	162.69(7)	C(21)	,	H(1)	84.72(10)
C(21)	,	H(101)	80.57(8)	C(21)	,	H(301)	83.43(8)	C(21)	,	H(5)	139.15(8)	C(21)	,	H(3)	158.98(9)
C(21)	,	H(12)	50.14(7)	C(21)	,	H(41)	70.93(7)	C(21)	,	H(601)	89.93(9)	C(21)	,	H(11)b	102.50(8)
C(21)	,	H(31)	27.45(6)	C(21)	,	H(401)a	124.41(8)	C(21)	,	H(2)	126.03(8)	C(21)	,	H(11)	25.54(7)
C(21)	,	H(23)	102.10(8)	O(5)	,	O(21)	85.76(6)	O(5)	,	C(31)	131.94(6)	O(5)	,	C(11)	126.51(6)
O(5)	,	C(2)	61.32(5)	O(5)	,	O(31)	144.31(6)	O(5)	,	O(11)	142.86(6)	O(5)	,	O(2)	90.75(5)

O(5)	,	C(5)	28.97(4)	O(5)	,	C(3)	63.95(5)	O(5)	,	C(41)	102.85(5)	O(5)	,	C(51)	87.14(5)
O(5)	,	O(41)a	98.25(5)	O(5)	,	C(4)	43.08(4)	O(5)	,	H(1)	53.78(8)	O(5)	,	H(101)	129.64(9)
O(5)	,	H(301)	128.34(8)	O(5)	,	H(5)	48.79(6)	O(5)	,	H(3)	80.32(7)	O(5)	,	H(12)	104.79(7)
O(5)	,	H(41)	90.83(6)	O(5)	,	H(601)	39.72(7)	O(5)	,	H(11)b	137.64(8)	O(5)	,	H(31)	136.73(7)
O(5)	,	H(401)a	101.66(8)	O(5)	,	H(2)	52.56(5)	O(5)	,	H(11)	129.15(8)	O(5)	,	H(23)	88.65(7)
O(21)	,	C(31)	59.13(5)	O(21)	,	C(11)	59.51(5)	O(21)	,	C(2)	120.46(6)	O(21)	,	O(31)	89.85(5)
O(21)	,	O(11)	89.91(6)	O(21)	,	O(2)	119.66(6)	O(21)	,	C(5)	108.95(5)	O(21)	,	C(3)	145.24(5)
O(21)	,	C(41)	50.10(4)	O(21)	,	C(51)	24.07(3)	O(21)	,	O(41)a	121.65(5)	O(21)	,	C(4)	128.83(5)
O(21)	,	H(1)	63.56(8)	O(21)	,	H(101)	105.58(8)	O(21)	,	H(301)	102.87(8)	O(21)	,	H(5)	114.13(7)
O(21)	,	H(3)	165.76(7)	O(21)	,	H(12)	58.38(7)	O(21)	,	H(41)	65.03(6)	O(21)	,	H(601)	58.34(8)
O(21)	,	H(11)b	136.61(7)	O(21)	,	H(31)	55.36(6)	O(21)	,	H(401)a	137.86(6)	O(21)	,	H(2)	109.09(6)
O(21)	,	H(11)	52.74(6)	O(21)	,	H(23)	106.52(7)	C(31)	,	C(11)	64.73(5)	C(31)	,	C(2)	164.01(6)
C(31)	,	O(31)	30.74(4)	C(31)	,	O(11)	73.99(5)	C(31)	,	O(2)	133.77(6)	C(31)	,	C(5)	131.77(5)
C(31)	,	C(3)	155.27(6)	C(31)	,	C(41)	29.68(3)	C(31)	,	C(51)	47.27(4)	C(31)	,	O(41)a	77.60(5)
C(31)	,	C(4)	150.72(5)	C(31)	,	H(1)	120.45(10)	C(31)	,	H(101)	93.23(8)	C(31)	,	H(301)	46.76(7)
C(31)	,	H(5)	114.21(7)	C(31)	,	H(3)	133.85(7)	C(31)	,	H(12)	84.80(7)	C(31)	,	H(41)	46.53(5)
C(31)	,	H(601)	92.24(7)	C(31)	,	H(11)b	83.36(7)	C(31)	,	H(31)	12.53(5)	C(31)	,	H(401)a	87.63(6)
C(31)	,	H(2)	163.05(7)	C(31)	,	H(11)	53.93(6)	C(31)	,	H(23)	129.93(7)	C(11)	,	C(2)	100.66(5)
C(11)	,	O(31)	79.64(5)	C(11)	,	O(11)	30.88(5)	C(11)	,	O(2)	76.08(5)	C(11)	,	C(5)	154.64(6)
C(11)	,	C(3)	125.21(5)	C(11)	,	C(41)	85.49(5)	C(11)	,	C(51)	76.30(5)	C(11)	,	O(41)a	133.82(5)
C(11)	,	C(4)	144.48(5)	C(11)	,	H(1)	73.82(8)	C(11)	,	H(101)	46.62(7)	C(11)	,	H(301)	100.05(7)
C(11)	,	H(5)	173.43(8)	C(11)	,	H(3)	127.90(7)	C(11)	,	H(12)	23.22(6)	C(11)	,	H(41)	106.55(7)
C(11)	,	H(601)	116.82(9)	C(11)	,	H(11)b	86.29(7)	C(11)	,	H(31)	52.20(5)	C(11)	,	H(401)a	131.63(7)
C(11)	,	H(2)	99.17(6)	C(11)	,	H(11)	11.36(6)	C(11)	,	H(23)	67.31(7)	C(2)	,	O(31)	145.41(6)
C(2)	,	O(11)	90.12(5)	C(2)	,	O(2)	30.56(4)	C(2)	,	C(5)	64.21(4)	C(2)	,	C(3)	30.29(4)
C(2)	,	C(41)	163.68(5)	C(2)	,	C(51)	138.81(5)	C(2)	,	O(41)a	111.71(6)	C(2)	,	C(4)	43.93(4)
C(2)	,	H(1)	56.92(8)	C(2)	,	H(101)	71.21(8)	C(2)	,	H(301)	136.65(8)	C(2)	,	H(5)	81.06(7)
C(2)	,	H(3)	49.33(6)	C(2)	,	H(12)	82.47(7)	C(2)	,	H(41)	149.42(7)	C(2)	,	H(601)	100.65(7)
C(2)	,	H(11)b	89.47(7)	C(2)	,	H(31)	152.14(6)	C(2)	,	H(401)a	98.69(7)	C(2)	,	H(2)	12.29(5)
C(2)	,	H(11)	111.83(7)	C(2)	,	H(23)	34.25(6)	O(31)	,	O(11)	72.37(5)	O(31)	,	O(2)	121.63(5)
O(31)	,	C(5)	124.67(5)	O(31)	,	C(3)	124.61(6)	O(31)	,	C(41)	50.32(4)	O(31)	,	C(51)	75.33(4)
O(31)	,	O(41)a	54.96(4)	O(31)	,	C(4)	129.40(5)	O(31)	,	H(1)	149.32(10)	O(31)	,	H(101)	85.61(8)
O(31)	,	H(301)	20.64(7)	O(31)	,	H(5)	102.60(7)	O(31)	,	H(3)	103.21(7)	O(31)	,	H(12)	102.81(7)
O(31)	,	H(41)	55.70(5)	O(31)	,	H(601)	110.09(7)	O(31)	,	H(11)b	55.95(7)	O(31)	,	H(31)	37.33(5)
O(31)	,	H(401)a	60.14(6)	O(31)	,	H(2)	157.49(6)	O(31)	,	H(11)	71.81(7)	O(31)	,	H(23)	126.35(7)
O(11)	,	O(2)	59.86(5)	O(11)	,	C(5)	153.28(6)	O(11)	,	C(3)	103.83(5)	O(11)	,	C(41)	102.35(5)
O(11)	,	C(51)	103.25(5)	O(11)	,	O(41)a	115.11(5)	O(11)	,	C(4)	128.71(5)	O(11)	,	H(1)	91.53(8)
O(11)	,	H(101)	20.28(7)	O(11)	,	H(301)	88.57(7)	O(11)	,	H(5)	155.67(8)	O(11)	,	H(3)	99.37(7)
O(11)	,	H(12)	44.24(6)	O(11)	,	H(41)	120.44(7)	O(11)	,	H(601)	147.70(9)	O(11)	,	H(11)b	56.92(7)
O(11)	,	H(31)	63.38(5)	O(11)	,	H(401)a	106.03(7)	O(11)	,	H(2)	94.95(6)	O(11)	,	H(11)	37.50(6)
O(11)	,	H(23)	57.38(6)	O(2)	,	C(5)	93.84(5)	O(2)	,	C(3)	49.14(4)	O(2)	,	C(41)	161.33(6)
O(2)	,	C(51)	143.72(6)	O(2)	,	O(41)a	118.47(6)	O(2)	,	C(4)	70.95(4)	O(2)	,	H(1)	66.41(8)
O(2)	,	H(101)	40.64(8)	O(2)	,	H(301)	124.60(7)	O(2)	,	H(5)	107.42(7)	O(2)	,	H(3)	57.99(6)
O(2)	,	H(12)	64.69(7)	O(2)	,	H(41)	175.16(8)	O(2)	,	H(601)	128.26(7)	O(2)	,	H(11)b	70.13(7)
O(2)	,	H(31)	123.08(6)	O(2)	,	H(401)a	101.83(6)	O(2)	,	H(2)	38.22(5)	O(2)	,	H(11)	87.34(7)
O(2)	,	H(23)	13.17(7)	C(5)	,	C(3)	50.14(4)	C(5)	,	C(41)	104.27(4)	C(5)	,	C(51)	101.28(4)
C(5)	,	O(41)a	71.47(4)	C(5)	,	C(4)	24.97(3)	C(5)	,	H(1)	80.83(8)	C(5)	,	H(101)	133.06(8)
C(5)	,	H(301)	104.75(7)	C(5)	,	H(5)	22.12(5)	C(5)	,	H(3)	58.88(6)	C(5)	,	H(12)	131.68(6)
C(5)	,	H(41)	85.35(6)	C(5)	,	H(601)	52.12(7)	C(5)	,	H(11)b	112.47(7)	C(5)	,	H(31)	143.08(6)

C(5)	, H(401)a	72.83(7)	C(5)	, H(2)	61.53(5)	C(5)	, H(11)	158.00(7)	C(5)	, H(23)	98.15(7)
C(3)	, C(41)	149.05(5)	C(3)	, C(51)	150.41(5)	C(3)	, O(41)a	81.43(5)	C(3)	, C(4)	25.18(3)
C(3)	, H(1)	84.00(8)	C(3)	, H(101)	83.67(7)	C(3)	, H(301)	109.15(8)	C(3)	, H(5)	58.64(6)
C(3)	, H(3)	21.42(5)	C(3)	, H(12)	111.20(7)	C(3)	, H(41)	127.99(7)	C(3)	, H(601)	100.48(7)
C(3)	, H(11)b	75.43(6)	C(3)	, H(31)	158.62(6)	C(3)	, H(401)a	69.05(6)	C(3)	, H(2)	39.04(5)
C(3)	, H(11)	136.40(6)	C(3)	, H(23)	58.93(6)	C(41)	, C(51)	27.99(3)	C(41)	, O(41)a	72.65(4)
C(41)	, C(4)	127.67(4)	C(41)	, H(1)	111.57(9)	C(41)	, H(101)	122.27(8)	C(41)	, H(301)	55.29(6)

C(41)	H(5)	91.22(6)	C(41)	H(3)	136.38(7)	C(41)	H(12)	99.05(7)	C(41)	H(41)	21.08(6)
C(41)	H(601)	63.26(6)	C(41)	H(11)b	106.11(7)	C(41)	H(31)	38.99(5)	C(41)	H(401)a	88.05(5)
C(41)	H(2)	152.18(6)	C(41)	H(11)	74.18(6)	C(41)	H(23)	151.88(8)	C(51)	O(41)a	97.64(4)
C(51)	C(4)	125.81(4)	C(51)	H(1)	83.59(8)	C(51)	H(101)	122.33(8)	C(51)	H(301)	83.18(7)
C(51)	H(5)	98.19(6)	C(51)	H(3)	155.54(7)	C(51)	H(12)	80.89(7)	C(51)	H(41)	40.96(6)
C(51)	H(601)	49.98(7)	C(51)	H(11)b	130.52(7)	C(51)	H(31)	49.59(5)	C(51)	H(401)a	114.06(5)
C(51)	H(2)	126.54(6)	C(51)	H(11)	66.74(6)	C(51)	H(23)	130.59(7)	O(41)a	C(4)	75.55(4)
O(41)a	H(1)	152.00(8)	O(41)a	H(101)	114.64(8)	O(41)a	H(301)	34.33(6)	O(41)a	H(5)	49.79(6)
O(41)a	H(3)	63.92(6)	O(41)a	H(12)	156.78(6)	O(41)a	H(41)	56.76(6)	O(41)a	H(601)	89.18(7)
O(41)a	H(11)b	62.83(6)	O(41)a	H(31)	88.72(5)	O(41)a	H(401)a	16.77(5)	O(41)a	H(2)	119.15(6)
O(41)a	H(11)	126.77(7)	O(41)a	H(23)	131.64(7)	C(4)	H(1)	81.09(8)	C(4)	H(101)	108.44(8)
C(4)	H(301)	109.27(7)	C(4)	H(5)	37.23(6)	C(4)	H(3)	37.34(5)	C(4)	H(12)	124.10(6)
C(4)	H(41)	107.33(6)	C(4)	H(601)	75.96(7)	C(4)	H(11)b	94.56(7)	C(4)	H(31)	163.19(6)
C(4)	H(401)a	69.41(6)	C(4)	H(2)	45.81(5)	C(4)	H(11)	155.35(6)	C(4)	H(23)	77.84(6)
H(1)	H(101)	87.19(10)	H(1)	H(301)	166.43(11)	H(1)	H(5)	102.25(9)	H(1)	H(3)	105.12(9)
H(1)	H(12)	51.18(8)	H(1)	H(41)	118.08(9)	H(1)	H(601)	70.12(9)	H(1)	H(11)b	135.29(9)
H(1)	H(31)	112.17(10)	H(1)	H(401)a	150.49(10)	H(1)	H(2)	45.65(9)	H(1)	H(11)	79.54(10)
H(1)	H(23)	55.40(9)	H(101)	H(301)	97.36(9)	H(101)	H(5)	139.29(10)	H(101)	H(3)	81.41(8)
H(101)	H(12)	50.88(9)	H(101)	H(41)	138.82(9)	H(101)	H(601)	156.18(10)	H(101)	H(11)b	51.82(9)
H(101)	H(31)	83.29(8)	H(101)	H(401)a	101.06(9)	H(101)	H(2)	77.78(8)	H(101)	H(11)	55.60(8)
H(101)	H(23)	40.99(9)	H(301)	H(5)	82.64(8)	H(301)	H(3)	88.24(8)	H(301)	H(12)	123.27(9)
H(301)	H(41)	51.28(7)	H(301)	H(601)	103.23(8)	H(301)	H(11)b	54.49(8)	H(301)	H(31)	56.10(8)
H(301)	H(401)a	41.01(8)	H(301)	H(2)	147.84(9)	H(301)	H(11)	92.45(9)	H(301)	H(23)	134.06(9)
H(5)	H(3)	57.88(8)	H(5)	H(12)	153.42(8)	H(5)	H(41)	70.39(7)	H(5)	H(601)	56.62(9)
H(5)	H(11)b	100.10(8)	H(5)	H(31)	126.65(7)	H(5)	H(401)a	53.76(8)	H(5)	H(2)	81.15(7)
H(5)	H(11)	164.69(8)	H(5)	H(23)	115.07(8)	H(3)	H(12)	122.54(9)	H(3)	H(41)	117.83(8)
H(3)	H(601)	110.79(9)	H(3)	H(11)b	57.40(8)	H(3)	H(31)	138.71(7)	H(3)	H(401)a	49.50(7)
H(3)	H(2)	59.63(7)	H(3)	H(11)	136.75(8)	H(3)	H(23)	70.37(8)	H(12)	H(41)	119.24(9)
H(12)	H(601)	106.70(9)	H(12)	H(11)b	100.46(8)	H(12)	H(31)	72.59(7)	H(12)	H(401)a	150.23(8)
H(12)	H(2)	78.37(7)	H(12)	H(11)	31.75(8)	H(12)	H(23)	52.93(8)	H(41)	H(601)	54.49(7)
H(41)	H(11)b	105.77(8)	H(41)	H(31)	57.86(6)	H(41)	H(401)a	73.36(7)	H(41)	H(2)	143.28(7)
H(41)	H(11)	95.21(8)	H(41)	H(23)	171.55(9)	H(601)	H(11)b	151.98(9)	H(601)	H(31)	98.29(8)
H(601)	H(401)a	102.32(8)	H(601)	H(2)	90.66(7)	H(601)	H(11)	111.07(9)	H(601)	H(23)	122.14(8)
H(11)b	H(31)	83.19(7)	H(11)b	H(401)a	49.99(8)	H(11)b	H(2)	101.58(8)	H(11)b	H(11)	88.61(8)
H(11)b	H(23)	80.08(8)	H(31)	H(401)a	97.00(7)	H(31)	H(2)	150.95(7)	H(31)	H(11)	41.45(7)
H(31)	H(23)	117.89(8)	H(401)a	H(2)	108.05(7)	H(401)a	H(11)	128.43(8)	H(401)a	H(23)	114.99(8)
H(2)	H(11)	109.61(7)	H(2)	H(23)	37.58(7)	H(11)	H(23)	78.66(8)			

3.6 Angstrom Coordination Sphere Around Atom I = O(2) [ARU = 1555.01]   0.22954 0.43550 0.74766   1.1941 3.7910 5.6533

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.972(3)	--	H(23)			Intra	-62.31	50.34	0.27190	0.37240	0.84660	1.4823	3.2417	6.4014
2	1.4247(16)	--	C(2)			Intra	17.32	-36.34	0.31253	0.47474	0.63600	2.2897	4.1326	4.8090
3	2.4175(19)	<<	C(3)			Intra	62.14	-34.96	0.28545	0.63673	0.56447	2.1199	5.5427	4.2681
4	2.4265(16)	<<	C(1)			Intra	-29.01	-54.98	0.29961	0.35792	0.48487	2.4120	3.1157	3.6663
5	2.781(2)	<<	O(11)			Intra	-138.18	-20.11	0.03017	0.23550	0.62119	-0.7519	2.0500	4.6970
6	2.8017(16)	<<	O(1)			Intra	-90.92	-73.91	0.17143	0.34630	0.39165	1.1816	3.0145	2.9614
7	2.855(2)	.<	O(61)a	x,y,1+z	1556.01		-72.44	50.83	0.32644	0.23800	1.04035	1.7381	2.0718	7.8664
8	2.893(2)	.<	O(3)			Intra	71.10	-6.73	0.30801	0.74770	0.70280	2.1245	6.5087	5.3141
9	3.231(2)	..	C(11)			Intra	-111.06	-28.50	0.10301	0.13110	0.54380	0.1739	1.1412	4.1118
10	3.4597(18)	..	C(31)b	-x,1/2+y,1-z	2556.01		139.88	4.70	-0.00718	0.69075	0.78515	-1.4426	6.0130	5.9368
11	3.5922(17)	..	C(21)			Intra	-102.88	-52.86	0.12446	0.19262	0.36895	0.7108	1.6768	2.7897
12	1.851(3)	<<	H(101)			Intra	-145.69	-22.44	0.08450	0.32470	0.65420	-0.2191	2.8265	4.9466
13	2.079(3)	<<	H(2)			Intra	8.21	-7.51	0.41160	0.46930	0.71170	3.2344	4.0853	5.3814
14	2.406(3)	<<	H(31)b	-x,1/2+y,1-z	2556.01		146.31	4.21	0.04950	0.58840	0.77100	-0.8023	5.1220	5.8298
15	2.669(3)	.<	H(3)			Intra	90.40	-46.95	0.18710	0.64480	0.48970	1.1814	5.6130	3.7028
16	2.740(3)	..	H(1)			Intra	-47.75	-35.20	0.33470	0.24510	0.53880	2.6995	2.1336	4.0740
17	2.877(4)	..	H(33)			Intra	89.34	-0.76	0.23180	0.76600	0.74260	1.2275	6.6680	5.6150
18	2.976(4)	..	H(12)			Intra	-93.61	-16.94	0.19470	0.10910	0.63300	1.0149	0.9497	4.7863
19	3.020(3)	..	H(61)a	x,y,1+z	1556.01		16.40	54.26	0.43720	0.49270	1.07190	2.8864	4.2890	8.1050
20	3.094(3)	..	H(41)a	x,y,1+z	1556.01		-143.91	40.89	0.09840	0.27720	1.01550	-0.6960	2.4130	7.6785
21	3.381(3)	..	H(11)b	-x,1/2+y,1-z	2556.01		163.72	-37.03	-0.05200	0.52240	0.47840	-1.3964	4.5475	3.6173
22	3.455(3)	..	H(601)a	x,y,1+z	1556.01		-67.55	64.57	0.34770	0.27800	1.16030	1.7605	2.4200	8.7734

Angles (Degrees) At1...V...At2 with Vertex V = O(2)

At1	At2	Angle	At1	At2	Angle	At1	At2	Angle	At1	At2	Angle
H(23)	C(2)	111.3(2)	H(23)	C(3)	137.5(2)	H(23)	C(1)	108.9(2)	H(23)	O(11)	96.8(2)
H(23)	O(1)	125.8(2)	H(23)	O(61)a	6.4(2)	H(23)	O(3)	121.7(2)	H(23)	C(11)	89.8(2)
H(23)	C(31)b	121.7(2)	H(23)	C(21)	108.7(2)	H(23)	H(101)	103.0(2)	H(23)	H(2)	83.7(2)
H(23)	H(31)b	120.2(2)	H(23)	H(3)	161.8(2)	H(23)	H(1)	86.5(2)	H(23)	H(33)	124.9(2)
H(23)	H(12)	72.7(2)	H(23)	H(61)a	45.7(2)	H(23)	H(41)a	54.9(2)	H(23)	H(11)b	144.8(2)
H(23)	H(601)a	14.50(19)	C(2)	C(3)	36.12(7)	C(2)	C(1)	36.43(6)	C(2)	O(11)	118.98(9)
C(2)	O(1)	60.03(6)	C(2)	O(61)a	117.21(9)	C(2)	O(3)	57.17(8)	C(2)	C(11)	99.02(8)
C(2)	C(31)b	118.73(10)	C(2)	C(21)	76.83(7)	C(2)	H(101)	119.06(12)	C(2)	H(2)	30.00(8)
C(2)	H(31)b	123.29(12)	C(2)	H(3)	53.63(8)	C(2)	H(1)	51.75(9)	C(2)	H(33)	75.14(11)
C(2)	H(12)	95.89(10)	C(2)	H(61)a	90.61(9)	C(2)	H(41)a	164.68(11)	C(2)	H(11)b	100.30(9)
C(2)	H(601)a	120.28(10)	C(3)	C(1)	62.63(4)	C(3)	O(11)	121.64(6)	C(3)	O(1)	69.64(5)
C(3)	O(61)a	143.86(7)	C(3)	O(3)	29.40(4)	C(3)	C(11)	116.22(5)	C(3)	C(31)b	82.73(5)
C(3)	C(21)	91.22(5)	C(3)	H(101)	116.82(10)	C(3)	H(2)	56.41(8)	C(3)	H(31)b	87.65(8)
C(3)	H(3)	24.28(6)	C(3)	H(1)	84.13(7)	C(3)	H(33)	42.56(7)	C(3)	H(12)	123.23(7)
C(3)	H(61)a	97.53(9)	C(3)	H(41)a	158.70(8)	C(3)	H(11)b	77.66(7)	C(3)	H(601)a	137.92(8)
C(1)	O(11)	84.00(5)	C(1)	O(1)	30.49(3)	C(1)	O(61)a	111.81(7)	C(1)	O(3)	90.23(5)
C(1)	C(11)	62.58(4)	C(1)	C(31)b	128.93(5)	C(1)	C(21)	41.49(3)	C(1)	H(101)	85.73(10)
C(1)	H(2)	55.93(7)	C(1)	H(31)b	129.09(8)	C(1)	H(3)	66.04(6)	C(1)	H(1)	23.63(5)

C(1)	H(33)	105.16(8)	C(1)	H(12)	61.70(6)	C(1)	H(61)a	115.43(8)	C(1)	H(41)a	135.95(8)
C(1)	H(11)b	87.35(7)	C(1)	H(601)a	123.15(8)	O(11)	O(1)	59.53(4)	O(11)	O(61)a	91.31(6)
O(11)	O(3)	140.63(7)	O(11)	C(11)	26.03(4)	O(11)	C(31)b	84.08(5)	O(11)	C(21)	42.54(4)
O(11)	H(101)	7.37(9)	O(11)	H(2)	136.91(10)	O(11)	H(31)b	77.93(8)	O(11)	H(3)	99.95(7)
O(11)	H(1)	78.90(7)	O(11)	H(33)	129.02(9)	O(11)	H(12)	42.26(6)	O(11)	H(61)a	140.76(10)
O(11)	H(41)a	61.23(6)	O(11)	H(11)b	52.89(6)	O(11)	H(601)a	100.19(8)	O(1)	O(61)a	125.37(7)

O(1)	O(3)	98.58(6)	O(1)	C(11)	46.60(4)	O(1)	C(31)b	104.67(5)	O(1)	C(21)	21.62(3)
O(1)	H(101)	59.03(9)	O(1)	H(2)	85.29(8)	O(1)	H(31)b	102.71(7)	O(1)	H(3)	59.14(6)
O(1)	H(1)	44.03(6)	O(1)	H(33)	105.33(8)	O(1)	H(12)	56.99(6)	O(1)	H(61)a	145.90(8)
O(1)	H(41)a	120.18(7)	O(1)	H(11)b	58.66(6)	O(1)	H(601)a	139.33(8)	O(61)a	O(3)	126.55(6)
O(61)a	C(11)	86.34(6)	O(61)a	C(31)b	117.94(5)	O(61)a	C(21)	106.81(6)	O(61)a	H(101)	97.33(10)
O(61)a	H(2)	89.98(9)	O(61)a	H(31)b	115.75(8)	O(61)a	H(3)	168.10(8)	O(61)a	H(1)	88.73(7)
O(61)a	H(33)	127.61(8)	O(61)a	H(12)	70.27(7)	O(61)a	H(61)a	50.45(9)	O(61)a	H(41)a	48.76(6)
O(61)a	H(11)b	138.39(8)	O(61)a	H(601)a	13.98(6)	O(3)	C(11)	144.71(6)	O(3)	C(31)b	69.59(5)
O(3)	C(21)	120.19(5)	O(3)	H(101)	133.66(11)	O(3)	H(2)	62.36(9)	O(3)	H(31)b	75.86(8)
O(3)	H(3)	43.49(6)	O(3)	H(1)	108.91(7)	O(3)	H(33)	19.14(7)	O(3)	H(12)	151.91(7)
O(3)	H(61)a	76.12(9)	O(3)	H(41)a	133.77(7)	O(3)	H(11)b	88.03(7)	O(3)	H(601)a	115.22(8)
C(11)	C(31)b	108.98(5)	C(11)	C(21)	25.10(3)	C(11)	H(101)	31.73(10)	C(11)	H(2)	111.32(9)
C(11)	H(31)b	103.10(8)	C(11)	H(3)	102.10(7)	C(11)	H(1)	53.30(6)	C(11)	H(33)	144.82(8)
C(11)	H(12)	19.77(5)	C(11)	H(61)a	134.38(10)	C(11)	H(41)a	75.77(6)	C(11)	H(11)b	69.77(6)
C(11)	H(601)a	99.04(7)	C(31)b	C(21)	109.92(4)	C(31)b	H(101)	77.53(10)	C(31)b	H(2)	131.89(10)
C(31)b	H(31)b	6.43(6)	C(31)b	H(3)	67.53(6)	C(31)b	H(1)	148.70(7)	C(31)b	H(33)	50.79(7)
C(31)b	H(12)	126.24(6)	C(31)b	H(61)a	104.75(8)	C(31)b	H(41)a	76.52(6)	C(31)b	H(11)b	47.28(5)
C(31)b	H(601)a	107.81(7)	C(21)	H(101)	44.46(9)	C(21)	H(2)	96.38(8)	C(21)	H(31)b	105.81(7)
C(21)	H(3)	79.55(6)	C(21)	H(1)	42.13(5)	C(21)	H(33)	125.41(8)	C(21)	H(12)	36.65(5)
C(21)	H(61)a	145.03(9)	C(21)	H(41)a	100.22(6)	C(21)	H(11)b	63.16(5)	C(21)	H(601)a	120.56(7)
H(101)	H(2)	140.62(13)	H(101)	H(31)b	71.51(12)	H(101)	H(3)	94.19(10)	H(101)	H(1)	83.35(11)
H(101)	H(33)	121.65(13)	H(101)	H(12)	49.11(11)	H(101)	H(61)a	145.44(12)	H(101)	H(41)a	63.35(9)
H(101)	H(11)b	45.71(10)	H(101)	H(601)a	105.26(11)	H(2)	H(31)b	138.21(12)	H(2)	H(3)	79.19(9)
H(2)	H(1)	58.07(9)	H(2)	H(33)	81.11(11)	H(2)	H(12)	98.98(10)	H(2)	H(61)a	62.16(9)
H(2)	H(41)a	138.42(10)	H(2)	H(11)b	129.90(10)	H(2)	H(601)a	90.77(9)	H(31)b	H(3)	70.85(9)
H(31)b	H(1)	146.39(9)	H(31)b	H(33)	57.14(10)	H(31)b	H(12)	119.97(9)	H(31)b	H(61)a	108.31(10)
H(31)b	H(41)a	72.03(8)	H(31)b	H(11)b	44.32(8)	H(31)b	H(601)a	106.82(9)	H(3)	H(1)	89.67(8)
H(3)	H(33)	46.20(8)	H(3)	H(12)	116.01(8)	H(3)	H(61)a	118.90(11)	H(3)	H(41)a	141.21(8)
H(3)	H(11)b	53.38(7)	H(3)	H(601)a	158.69(9)	H(1)	H(33)	126.21(10)	H(1)	H(12)	44.57(7)
H(1)	H(61)a	105.05(9)	H(1)	H(41)a	116.33(9)	H(1)	H(11)b	102.08(8)	H(1)	H(601)a	100.98(9)
H(33)	H(12)	162.06(9)	H(33)	H(61)a	80.76(11)	H(33)	H(41)a	117.46(9)	H(33)	H(11)b	77.12(9)
H(33)	H(601)a	114.01(9)	H(12)	H(61)a	115.32(11)	H(12)	H(41)a	74.26(7)	H(12)	H(11)b	89.54(7)
H(12)	H(601)a	83.92(8)	H(61)a	H(41)a	83.36(8)	H(61)a	H(11)b	151.80(10)	H(61)a	H(601)a	40.58(10)
H(41)a	H(11)b	91.48(8)	H(41)a	H(601)a	48.11(7)	H(11)b	H(601)a	139.32(9)			

3.6 Angstrom Coordination Sphere Around Atom I = O(3) [ARU = 1555.01]   0.30801 0.74770 0.70280   2.1245 6.5087 5.3141

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.960(4)	--	H(33)	[	=]	Intra	169.93	18.28	0.23180	0.76600	0.74260	1.2275	6.6680	5.6150
2	1.424(2)	--	C(3)	[	=]	Intra	-90.28	-47.28	0.28545	0.63673	0.56447	2.1199	5.5427	4.2681
3	2.3887(19)	<<	C(4)	[	=]	Intra	-29.71	-55.65	0.37404	0.67095	0.44198	3.2951	5.8406	3.3420
4	2.435(2)	<<	C(2)	[	=]	Intra	-86.02	-11.97	0.31253	0.47474	0.63600	2.2897	4.1326	4.8090
5	2.849(2)	.<	O(6)d	[1-x,1/2+y,1-z	= 2656.01]		65.48	1.67	0.41856	1.04530	0.71380	3.3063	9.0993	5.3973
6	2.8618(19)	.<	O(31)e	[-x,1/2+y,1-z	= 2556.01]		167.30	14.17	0.07367	0.81776	0.79548	-0.5823	7.1186	6.0149
7	2.879(2)	.<	O(4)	[	=]	Intra	28.94	-65.49	0.34880	0.81410	0.35630	3.1699	7.0867	2.6941
8	2.893(2)	.<	O(2)	[	=]	Intra	-108.90	6.73	0.22954	0.43550	0.74766	1.1941	3.7910	5.6533
9	1.921(4)	<<	H(63)d	[1-x,1/2+y,1-z	= 2656.01]		59.83	2.39	0.39850	0.93830	0.71340	3.0891	8.1679	5.3942
10	2.071(3)	<<	H(3)	[	=]	Intra	-136.48	-51.09	0.18710	0.64480	0.48970	1.1814	5.6130	3.7028
11	2.534(5)	.<	H(43)	[	=]	Intra	56.58	-53.77	0.34070	0.89130	0.43250	2.9494	7.7588	3.2703
12	2.595(3)	.<	H(4)	[	=]	Intra	-18.32	-31.83	0.47170	0.66810	0.52180	4.2173	5.8158	3.9455
13	2.666(3)	.<	H(2)	[	=]	Intra	-65.39	1.45	0.41160	0.46930	0.71170	3.2344	4.0853	5.3814
14	3.105(4)	..	H(62)c	[x,1+y,1+z	= 1566.01]		108.04	30.51	0.26510	1.03990	0.91130	1.2960	9.0523	6.8906
15	3.279(3)	..	H(31)e	[-x,1/2+y,1-z	= 2556.01]		-154.65	9.05	0.04950	0.58840	0.77100	-0.8023	5.1220	5.8298
16	3.377(4)	..	H(12)b	[x,1+y,z	= 1565.01]		109.43	-8.99	0.19470	1.10910	0.63300	1.0149	9.6547	4.7863
17	3.408(3)	..	H(6)a	[x,y,1+z	= 1556.01]		-32.48	73.30	0.45310	0.68730	1.13450	2.9504	5.9829	8.5783
18	3.503(4)	..	H(23)	[	=]	Intra	-101.12	18.09	0.27190	0.37240	0.84660	1.4823	3.2417	6.4014

Angles (Degrees) At1...V...At2 with Vertex V = O(3)

At1 , At2	Angle	At1 , At2	Angle	At1 , At2	Angle	At1 , At2	Angle
H(33) , C(3)	109.9(2)	H(33) , C(4)	139.8(2)	H(33) , C(2)	106.9(2)	H(33) , O(6)d	103.2(2)
H(33) , O(31)e	4.8(2)	H(33) , O(4)	126.3(2)	H(33) , O(2)	79.5(2)	H(33) , H(63)d	108.2(3)
H(33) , H(3)	83.7(2)	H(33) , H(43)	118.4(3)	H(33) , H(4)	164.5(2)	H(33) , H(2)	122.1(2)
H(33) , H(62)c	57.0(2)	H(33) , H(31)e	35.6(2)	H(33) , H(12)b	65.6(2)	H(33) , H(6)a	87.2(2)
H(33) , H(23)	83.5(2)	C(3) , C(4)	37.38(6)	C(3) , C(2)	35.48(7)	C(3) , O(6)d	129.78(10)
C(3) , O(31)e	108.75(9)	C(3) , O(4)	57.92(8)	C(3) , O(2)	56.47(8)	C(3) , H(63)d	128.19(15)
C(3) , H(3)	29.93(8)	C(3) , H(43)	75.12(12)	C(3) , H(4)	55.53(8)	C(3) , H(2)	53.36(9)
C(3) , H(62)c	158.11(11)	C(3) , H(31)e	79.96(9)	C(3) , H(12)b	121.07(10)	C(3) , H(6)a	126.85(11)
C(3) , H(23)	66.09(9)	C(4) , C(2)	61.48(5)	C(4) , O(6)d	94.31(7)	C(4) , O(31)e	136.49(7)
C(4) , O(4)	29.19(5)	C(4) , O(2)	89.52(6)	C(4) , H(63)d	91.72(13)	C(4) , H(3)	57.30(8)
C(4) , H(43)	46.57(10)	C(4) , H(4)	25.12(6)	C(4) , H(2)	64.06(7)	C(4) , H(62)c	141.17(9)
C(4) , H(31)e	116.67(8)	C(4) , H(12)b	107.01(7)	C(4) , H(6)a	128.97(8)	C(4) , H(23)	94.89(7)
C(2) , O(6)d	149.93(7)	C(2) , O(31)e	108.84(7)	C(2) , O(4)	89.00(6)	C(2) , O(2)	29.45(4)
C(2) , H(63)d	144.84(13)	C(2) , H(3)	56.45(8)	C(2) , H(43)	106.98(11)	C(2) , H(4)	64.87(7)
C(2) , H(2)	24.50(6)	C(2) , H(62)c	157.34(9)	C(2) , H(31)e	71.37(6)	C(2) , H(12)b	154.01(8)
C(2) , H(6)a	91.82(8)	C(2) , H(23)	33.55(5)	O(6)d , O(31)e	101.04(7)	O(6)d , O(4)	72.15(6)
O(6)d , O(2)	169.89(7)	O(6)d , H(63)d	5.69(11)	O(6)d , H(3)	127.23(10)	O(6)d , H(43)	55.93(10)
O(6)d , H(4)	85.62(8)	O(6)d , H(2)	130.78(8)	O(6)d , H(62)c	49.53(7)	O(6)d , H(31)e	138.61(8)
O(6)d , H(12)b	45.07(6)	O(6)d , H(6)a	90.68(8)	O(6)d , H(23)	156.24(8)	O(31)e , O(4)	121.56(7)
O(31)e , O(2)	82.37(6)	O(31)e , H(63)d	106.30(12)	O(31)e , H(3)	81.49(8)	O(31)e , H(43)	113.60(15)
O(31)e , H(4)	161.61(8)	O(31)e , H(2)	125.54(8)	O(31)e , H(62)c	56.55(7)	O(31)e , H(31)e	37.58(6)
O(31)e , H(12)b	61.90(6)	O(31)e , H(6)a	91.58(7)	O(31)e , H(23)	87.10(7)	O(4) , O(2)	114.34(7)

O(4) ,	H(63)d	71.47(13)	O(4) ,	H(3)	62.88(8)	O(4) ,	H(43)	17.98(9)	O(4) ,	H(4)	44.02(7)
O(4) ,	H(2)	93.11(8)	O(4) ,	H(62)c	113.23(9)	O(4) ,	H(31)e	123.50(7)	O(4) ,	H(12)b	77.88(6)
O(4) ,	H(6)a	144.54(9)	O(4) ,	H(23)	122.43(7)	O(2) ,	H(63)d	165.51(13)	O(2) ,	H(3)	62.51(8)
O(2) ,	H(43)	131.52(11)	O(2) ,	H(4)	94.04(8)	O(2) ,	H(2)	43.69(6)	O(2) ,	H(62)c	128.63(8)
O(2) ,	H(31)e	45.35(6)	O(2) ,	H(12)b	141.98(7)	O(2) ,	H(6)a	79.67(7)	O(2) ,	H(23)	13.65(5)
H(63)d ,	H(3)	129.41(15)	H(63)d ,	H(43)	56.22(16)	H(63)d ,	H(4)	81.24(13)	H(63)d ,	H(2)	125.10(13)

H(63)d ,	H(62)c	53.50(13)	H(63)d ,	H(31)e	143.79(13)	H(63)d ,	H(12)b	50.72(12)	H(63)d ,	H(6)a	88.37(14)
H(63)d ,	H(23)	152.23(14)	H(3) ,	H(43)	74.58(14)	H(3) ,	H(4)	80.87(10)	H(3) ,	H(2)	79.40(10)
H(3) ,	H(62)c	128.89(11)	H(3) ,	H(31)e	62.16(8)	H(3) ,	H(12)b	97.57(10)	H(3) ,	H(6)a	142.09(11)
H(3) ,	H(23)	75.79(9)	H(43) ,	H(4)	56.20(14)	H(43) ,	H(2)	109.47(13)	H(43) ,	H(62)c	95.29(12)
H(43) ,	H(31)e	128.75(15)	H(43) ,	H(12)b	61.40(12)	H(43) ,	H(6)a	140.34(15)	H(43) ,	H(23)	140.38(11)
H(4) ,	H(2)	55.59(8)	H(4) ,	H(62)c	134.57(10)	H(4) ,	H(31)e	133.62(9)	H(4) ,	H(12)b	115.55(9)
H(4) ,	H(6)a	105.58(9)	H(4) ,	H(23)	93.59(9)	H(2) ,	H(62)c	147.44(10)	H(2) ,	H(31)e	89.04(8)
H(2) ,	H(12)b	170.86(8)	H(2) ,	H(6)a	74.62(8)	H(2) ,	H(23)	38.80(8)	H(62)c ,	H(31)e	91.63(8)
H(62)c ,	H(12)b	39.52(7)	H(62)c ,	H(6)a	72.83(9)	H(62)c ,	H(23)	123.89(9)	H(31)e ,	H(12)b	97.19(7)
H(31)e ,	H(6)a	90.02(8)	H(31)e ,	H(23)	52.64(7)	H(12)b ,	H(6)a	111.90(8)	H(12)b ,	H(23)	148.99(8)
H(6)a ,	H(23)	66.62(8)									

3.6 Angstrom Coordination Sphere Around Atom I = O(4) [ARU = 1555.01]   0.34880 0.81410 0.35630   3.1699 7.0867 2.6941

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.912(4)	--	H(43)	[	=]	Intra	108.16	39.17	0.34070	0.89130	0.43250	2.9494	7.7588	3.2703
2	1.410(2)	--	C(4)	[	=]	Intra	-84.26	27.35	0.37404	0.67095	0.44198	3.2951	5.8406	3.3420
3	2.346(2)	<<	C(5)	[	=]	Intra	-84.52	-11.34	0.35925	0.55107	0.29529	3.3894	4.7971	2.2328
4	2.442(2)	<<	C(3)	[	=]	Intra	-124.22	40.13	0.28545	0.63673	0.56447	2.1199	5.5427	4.2681
5	2.838(2)	<<	O(21)a	[x,1+y,z	= 1565.01]		120.11	-6.21	0.21205	1.09445	0.31572	1.7548	9.5272	2.3873
6	2.879(2)	.<	O(3)	[	=]	Intra	-151.06	65.49	0.30801	0.74770	0.70280	2.1245	6.5087	5.3141
7	2.891(2)	<<	C(6)	[	=]	Intra	-55.05	-26.69	0.45754	0.57083	0.18455	4.6496	4.9691	1.3954
8	3.127(2)	.<	C(51)a	[x,1+y,z	= 1565.01]		124.47	-33.40	0.17635	1.06133	0.12864	1.6922	9.2389	0.9727
9	3.306(2)	..	C(61)a	[x,1+y,z	= 1565.01]		92.67	-45.09	0.28927	1.08194	0.04668	3.0613	9.4183	0.3530
10	3.333(2)	..	O(5)b	[1-x,1/2+y,1-z	= 2656.01]		16.44	38.60	0.62281	0.89878	0.63136	5.6685	7.8239	4.7739
11	3.373(2)	..	O(6)b	[1-x,1/2+y,1-z	= 2656.01]		86.12	53.27	0.41856	1.04530	0.71380	3.3063	9.0993	5.3973
12	3.574(2)	..	O(6)	[	=]	Intra	-41.45	-8.53	0.58144	0.54530	0.28620	5.8189	4.7468	2.1641
13	2.068(3)	<<	H(4)	[	=]	Intra	-50.51	37.23	0.47170	0.66810	0.52180	4.2173	5.8158	3.9455
14	2.517(4)	<<	H(6)	[	=]	Intra	-36.01	-41.78	0.45310	0.68730	0.13450	4.6884	5.9829	1.0170
15	2.554(3)	.<	H(5)	[	=]	Intra	-106.88	-25.80	0.26380	0.56130	0.20930	2.5020	4.8861	1.5826
16	2.558(4)	.<	H(611)a	[x,1+y,z	= 1565.01]		70.45	-44.42	0.36720	1.01190	0.11950	3.7813	8.8086	0.9036
17	2.673(3)	.<	H(3)	[	=]	Intra	-143.46	22.17	0.18710	0.64480	0.48970	1.1814	5.6130	3.7028
18	2.780(3)	..	H(51)a	[x,1+y,z	= 1565.01]		148.29	-41.36	0.14650	0.94010	0.11330	1.3946	8.1836	0.8567
19	2.910(4)	..	H(63)b	[1-x,1/2+y,1-z	= 2656.01]		94.27	68.12	0.39850	0.93830	0.71340	3.0891	8.1679	5.3942
20	3.081(3)	..	H(2)b	[1-x,1/2+y,1-z	= 2656.01]		26.40	-9.61	0.58840	0.96930	0.28830	5.8909	8.4378	2.1799
21	3.405(3)	..	H(1)b	[1-x,1/2+y,1-z	= 2656.01]		-10.45	13.47	0.66530	0.74510	0.46120	6.4258	6.4861	3.4873
22	3.533(4)	..	H(33)	[	=]	Intra	-167.84	55.77	0.23180	0.76600	0.74260	1.2275	6.6680	5.6150

Angles (Degrees) At1...V...At2 with Vertex V = O(4)

H(43)	C(4)	112.5(3)	H(43)	C(5)	150.0(3)	H(43)	C(3)	87.4(3)	H(43)	O(21)a	46.7(3)
H(43)	O(3)	59.0(3)	H(43)	C(6)	161.2(4)	H(43)	C(51)a	74.1(3)	H(43)	C(61)a	85.4(3)
H(43)	O(5)b	67.9(4)	H(43)	O(6)b	20.6(4)	H(43)	O(6)	139.0(4)	H(43)	H(4)	101.1(3)
H(43)	H(6)	152.8(4)	H(43)	H(5)	147.8(4)	H(43)	H(611)a	90.2(3)	H(43)	H(3)	89.3(4)
H(43)	H(51)a	88.4(4)	H(43)	H(63)b	29.9(3)	H(43)	H(2)b	89.8(4)	H(43)	H(1)b	102.4(4)
H(43)	H(33)	55.4(3)	C(4)	C(5)	38.69(7)	C(4)	C(3)	35.25(7)	C(4)	O(21)a	148.65(12)
C(4)	O(3)	55.72(8)	C(4)	C(6)	60.90(8)	C(4)	C(51)a	154.57(12)	C(4)	C(61)a	162.10(10)
C(4)	O(5)b	80.92(9)	C(4)	O(6)b	98.95(9)	C(4)	O(6)	54.81(8)	C(4)	H(4)	30.01(9)
C(4)	H(6)	82.24(12)	C(4)	H(5)	57.44(9)	C(4)	H(611)a	153.53(14)	C(4)	H(3)	53.52(9)
C(4)	H(51)a	135.15(13)	C(4)	H(63)b	84.52(11)	C(4)	H(2)b	112.69(12)	C(4)	H(1)b	69.64(10)
C(4)	H(33)	64.16(9)	C(5)	C(3)	63.25(6)	C(5)	O(21)a	149.86(9)	C(5)	O(3)	90.97(7)
C(5)	C(6)	31.68(4)	C(5)	C(51)a	127.42(7)	C(5)	C(61)a	123.52(7)	C(5)	O(5)b	105.57(7)
C(5)	O(6)b	137.41(7)	C(5)	O(6)	42.48(5)	C(5)	H(4)	58.12(9)	C(5)	H(6)	52.02(9)
C(5)	H(5)	25.58(6)	C(5)	H(611)a	119.80(11)	C(5)	H(3)	66.78(7)	C(5)	H(51)a	108.35(8)
C(5)	H(63)b	123.21(10)	C(5)	H(2)b	108.21(9)	C(5)	H(1)b	77.53(7)	C(5)	H(33)	95.65(8)
C(3)	O(21)a	113.52(8)	C(3)	O(3)	29.60(5)	C(3)	C(6)	92.66(7)	C(3)	C(51)a	125.93(8)
C(3)	C(61)a	152.65(8)	C(3)	O(5)b	93.44(6)	C(3)	O(6)b	83.00(6)	C(3)	O(6)	90.02(6)
C(3)	H(4)	55.90(8)	C(3)	H(6)	114.30(11)	C(3)	H(5)	67.87(7)	C(3)	H(611)a	168.35(12)

C(3) ,	H(3)	24.25(6)	C(3) ,	H(51)a	113.63(10)	C(3) ,	H(63)b	67.97(8)	C(3) ,	H(2)b	139.86(9)
C(3) ,	H(1)b	98.60(7)	C(3) ,	H(33)	32.41(7)	O(21)a ,	O(3)	95.16(6)	O(21)a ,	C(6)	146.77(7)
O(21)a ,	C(51)a	27.49(3)	O(21)a ,	C(61)a	45.61(4)	O(21)a ,	O(5)b	104.54(6)	O(21)a ,	O(6)b	66.03(5)
O(21)a ,	O(6)	156.44(7)	O(21)a ,	H(4)	147.82(10)	O(21)a ,	H(6)	127.29(10)	O(21)a ,	H(5)	124.30(9)
O(21)a ,	H(611)a	57.63(9)	O(21)a ,	H(3)	98.28(8)	O(21)a ,	H(51)a	43.19(6)	O(21)a ,	H(63)b	76.52(8)
O(21)a ,	H(2)b	92.59(7)	O(21)a ,	H(1)b	130.83(8)	O(21)a ,	H(33)	85.25(7)	O(3) ,	C(6)	116.58(7)

O(3)	C(51)a	117.87(7)	O(3)	C(61)a	140.72(7)	O(3)	O(5)b	75.45(5)	O(3)	O(6)b	53.50(5)
O(3)	O(6)	105.82(6)	O(3)	H(4)	60.66(8)	O(3)	H(6)	137.49(11)	O(3)	H(5)	97.36(8)
O(3)	H(611)a	149.17(11)	O(3)	H(3)	43.60(6)	O(3)	H(51)a	116.66(9)	O(3)	H(63)b	38.75(8)
O(3)	H(2)b	124.09(8)	O(3)	H(1)b	95.73(7)	O(3)	H(33)	12.65(6)	C(6)	C(51)a	119.91(6)
C(6)	C(61)a	102.43(6)	C(6)	O(5)b	93.36(6)	C(6)	O(6)b	140.92(7)	C(6)	O(6)	22.27(4)
C(6)	H(4)	64.06(8)	C(6)	H(6)	21.71(8)	C(6)	H(5)	46.16(6)	C(6)	H(611)a	93.23(10)
C(6)	H(3)	98.42(8)	C(6)	H(51)a	108.59(8)	C(6)	H(63)b	134.68(10)	C(6)	H(2)b	78.13(7)
C(6)	H(1)b	59.07(6)	C(6)	H(33)	124.47(8)	C(51)a	C(61)a	27.03(3)	C(51)a	O(5)b	123.06(6)
C(51)a	O(6)b	92.85(6)	C(51)a	O(6)	135.99(6)	C(51)a	H(4)	174.40(11)	C(51)a	H(6)	102.71(9)
C(51)a	H(5)	103.29(8)	C(51)a	H(611)a	42.65(8)	C(51)a	H(3)	103.63(8)	C(51)a	H(51)a	20.45(6)
C(51)a	H(63)b	104.00(9)	C(51)a	H(2)b	91.36(7)	C(51)a	H(1)b	134.55(8)	C(51)a	H(33)	106.08(8)
C(61)a	O(5)b	108.09(6)	C(61)a	O(6)b	98.51(6)	C(61)a	O(6)	112.40(6)	C(61)a	H(4)	151.45(11)
C(61)a	H(6)	81.79(9)	C(61)a	H(5)	106.91(8)	C(61)a	H(611)a	15.74(8)	C(61)a	H(3)	129.18(9)
C(61)a	H(51)a	39.90(7)	C(61)a	H(63)b	113.22(9)	C(61)a	H(2)b	66.52(6)	C(61)a	H(1)b	108.71(7)
C(61)a	H(33)	130.62(8)	O(5)b	O(6)b	48.52(4)	O(5)b	O(6)	71.44(5)	O(5)b	H(4)	51.60(8)
O(5)b	H(6)	93.47(10)	O(5)b	H(5)	131.15(9)	O(5)b	H(611)a	96.24(10)	O(5)b	H(3)	116.37(7)
O(5)b	H(51)a	143.48(9)	O(5)b	H(63)b	50.18(7)	O(5)b	H(2)b	49.10(6)	O(5)b	H(1)b	34.60(5)
O(5)b	H(33)	85.55(7)	O(6)b	O(6)	118.65(6)	O(6)b	H(4)	82.03(9)	O(6)b	H(6)	140.46(11)
O(6)b	H(5)	150.86(9)	O(6)b	H(611)a	98.61(10)	O(6)b	H(3)	93.25(7)	O(6)b	H(51)a	108.67(8)
O(6)b	H(63)b	15.35(8)	O(6)b	H(2)b	80.58(7)	O(6)b	H(1)b	83.10(6)	O(6)b	H(33)	55.27(7)
O(6)	H(4)	46.54(8)	O(6)	H(6)	33.59(8)	O(6)	H(5)	64.23(7)	O(6)	H(611)a	99.19(10)
O(6)	H(3)	104.26(8)	O(6)	H(51)a	129.31(8)	O(6)	H(63)b	113.67(9)	O(6)	H(2)b	66.91(7)
O(6)	H(1)b	37.83(5)	O(6)	H(33)	116.91(8)	H(4)	H(6)	80.11(11)	H(4)	H(5)	82.32(10)
H(4)	H(611)a	135.72(13)	H(4)	H(3)	79.02(10)	H(4)	H(51)a	164.91(12)	H(4)	H(63)b	71.39(11)
H(4)	H(2)b	85.59(10)	H(4)	H(1)b	42.81(9)	H(4)	H(33)	72.87(9)	H(6)	H(5)	59.34(10)
H(6)	H(611)a	71.62(12)	H(6)	H(3)	117.29(12)	H(6)	H(51)a	96.77(10)	H(6)	H(63)b	142.93(13)
H(6)	H(2)b	63.15(10)	H(6)	H(1)b	60.06(9)	H(6)	H(33)	146.16(12)	H(5)	H(611)a	109.74(11)
H(5)	H(3)	59.64(8)	H(5)	H(51)a	83.42(9)	H(5)	H(63)b	135.78(11)	H(5)	H(2)b	122.42(9)
H(5)	H(1)b	101.50(9)	H(5)	H(33)	96.54(9)	H(611)a	H(3)	144.40(12)	H(611)a	H(51)a	54.87(10)
H(611)a	H(63)b	113.96(12)	H(611)a	H(2)b	51.47(9)	H(611)a	H(1)b	93.05(10)	H(611)a	H(33)	142.17(12)
H(3)	H(51)a	89.54(10)	H(3)	H(63)b	80.45(9)	H(3)	H(2)b	164.11(9)	H(3)	H(1)b	121.76(9)
H(3)	H(33)	38.14(8)	H(51)a	H(63)b	116.68(11)	H(51)a	H(2)b	106.30(9)	H(51)a	H(1)b	146.53(10)
H(51)a	H(33)	104.01(10)	H(63)b	H(2)b	90.94(9)	H(63)b	H(1)b	82.87(9)	H(63)b	H(33)	42.40(9)
H(2)b	H(1)b	43.25(7)	H(2)b	H(33)	132.49(9)	H(1)b	H(33)	108.20(8)			

3.6 Angstrom Coordination Sphere Around Atom I = O(5) [ARU = 1555.01]   0.37719 0.39878 0.36864   3.4568 3.4714 2.7874

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J		ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	1.4108(14)	--	C(1)	[	=	]	Intra	-161.20	38.53	0.29961	0.35792	0.48487	2.4120	3.1157	3.6663
2	1.4386(19)	--	C(5)	[	=	]	Intra	92.91	-22.68	0.35925	0.55107	0.29529	3.3894	4.7971	2.2328
3	2.3271(15)	<<	O(1)	[	=	]	Intra	-168.65	4.29	0.17143	0.34630	0.39165	1.1816	3.0145	2.9614
4	2.3672(18)	<<	C(6)	[	=	]	Intra	51.46	-36.02	0.45754	0.57083	0.18455	4.6496	4.9691	1.3954
5	2.4261(15)	<<	C(2)	[	=	]	Intra	150.47	56.43	0.31253	0.47474	0.63600	2.2897	4.1326	4.8090
6	2.4386(19)	<<	C(4)	[	=	]	Intra	93.90	13.14	0.37404	0.67095	0.44198	3.2951	5.8406	3.3420
7	2.7559(19)	<<	O(6)	[	=	]	Intra	28.37	-13.07	0.58144	0.54530	0.28620	5.8189	4.7468	2.1641
8	2.8497(19)	.<	O(61)	[	=	]	Intra	-89.21	-60.58	0.32644	0.23800	0.04035	3.4761	2.0718	0.3051
9	2.8759(17)	<<	C(3)	[	=	]	Intra	122.84	30.99	0.28545	0.63673	0.56447	2.1199	5.5427	4.2681
10	3.1741(19)	..	O(21)	[	=	]	Intra	-122.72	-7.24	0.21205	0.09445	0.31572	1.7548	0.8222	2.3873
11	3.2804(16)	..	C(21)	[	=	]	Intra	-146.83	0.04	0.12446	0.19262	0.36895	0.7108	1.6768	2.7897
12	3.333(2)	..	O(4)a	[1-x,-1/2+y,1-z	=	2646.01]		-16.44	38.60	0.65120	0.31410	0.64370	5.9554	2.7342	4.8672
13	3.4083(17)	..	C(4)a	[1-x,-1/2+y,1-z	=	2646.01]		-39.88	24.84	0.62596	0.17095	0.55802	5.8301	1.4881	4.2194
14	1.894(3)	<<	H(601)	[	=	]	Intra	-87.73	-56.26	0.34770	0.27800	0.16030	3.4986	2.4200	1.2121
15	2.005(3)	<<	H(1)	[	=	]	Intra	-119.51	39.93	0.33470	0.24510	0.53880	2.6995	2.1336	4.0740
16	2.089(3)	<<	H(5)	[	=	]	Intra	124.02	-35.22	0.26380	0.56130	0.20930	2.5020	4.8861	1.5826
17	2.612(3)	.<	H(4)a	[1-x,-1/2+y,1-z	=	2646.01]		-54.15	18.49	0.52830	0.16810	0.47820	4.9080	1.4633	3.6158
18	2.658(3)	.<	H(61)	[	=	]	Intra	35.00	-57.57	0.43720	0.49270	0.07190	4.6245	4.2890	0.5437
19	2.675(3)	.<	H(2)	[	=	]	Intra	109.92	75.87	0.41160	0.46930	0.71170	3.2344	4.0853	5.3814
20	2.675(4)	.<	H(63)	[	=	]	Intra	7.60	-13.41	0.60150	0.43830	0.28660	6.0362	3.8154	2.1671
21	2.723(3)	..	H(4)	[	=	]	Intra	72.03	25.17	0.47170	0.66810	0.52180	4.2173	5.8158	3.9455
22	3.108(6)	..	H(43)a	[1-x,-1/2+y,1-z	=	2646.01]		-1.37	28.94	0.65930	0.39130	0.56750	6.1758	3.4063	4.2910
23	3.256(3)	..	H(3)	[	=	]	Intra	136.74	16.33	0.18710	0.64480	0.48970	1.1814	5.6130	3.7028
24	3.310(4)	..	H(6)	[	=	]	Intra	63.88	-32.33	0.45310	0.68730	0.13450	4.6884	5.9829	1.0170

Angles (Degrees) At1...V...At2 with Vertex V = O(5)

C(1)	C(5)	115.96(9)	C(1)	O(1)	34.91(5)	C(1)	C(6)	154.02(9)	C(1)	C(2)	36.24(5)
C(1)	C(4)	93.11(7)	C(1)	O(6)	153.16(8)	C(1)	O(61)	115.07(8)	C(1)	C(3)	61.09(5)
C(1)	O(21)	58.06(5)	C(1)	C(21)	40.69(5)	C(1)	O(4)a	96.35(7)	C(1)	C(4)a	96.16(7)
C(1)	H(601)	113.23(13)	C(1)	H(1)	32.03(8)	C(1)	H(5)	101.04(9)	C(1)	H(4)a	91.15(8)
C(1)	H(61)	158.22(11)	C(1)	H(2)	52.57(7)	C(1)	H(63)	152.99(11)	C(1)	H(4)	99.15(8)
C(1)	H(43)a	109.95(11)	C(1)	H(3)	58.21(6)	C(1)	H(6)	143.12(10)	C(5)	O(1)	99.43(8)
C(5)	C(6)	38.18(6)	C(5)	C(2)	92.73(8)	C(5)	C(4)	35.83(6)	C(5)	O(6)	61.74(7)
C(5)	O(61)	96.72(8)	C(5)	C(3)	60.86(6)	C(5)	O(21)	134.06(8)	C(5)	C(21)	117.72(7)
C(5)	O(4)a	118.65(8)	C(5)	C(4)a	136.96(8)	C(5)	H(601)	101.06(12)	C(5)	H(1)	147.64(11)
C(5)	H(5)	29.80(8)	C(5)	H(4)a	148.94(9)	C(5)	H(61)	53.97(11)	C(5)	H(2)	99.12(9)
C(5)	H(63)	80.63(10)	C(5)	H(4)	51.95(8)	C(5)	H(43)a	104.29(10)	C(5)	H(3)	57.96(7)
C(5)	H(6)	27.39(8)	O(1)	C(6)	131.36(7)	O(1)	C(2)	61.37(5)	O(1)	C(4)	96.25(6)
O(1)	O(6)	161.04(7)	O(1)	O(61)	88.59(5)	O(1)	C(3)	69.41(5)	O(1)	O(21)	47.26(5)
O(1)	C(21)	22.20(4)	O(1)	O(4)a	130.00(6)	O(1)	C(4)a	122.35(6)	O(1)	H(601)	88.55(11)
O(1)	H(1)	56.75(8)	O(1)	H(5)	74.29(8)	O(1)	H(4)a	111.62(8)	O(1)	H(61)	123.57(9)
O(1)	H(2)	83.76(6)	O(1)	H(63)	170.15(10)	O(1)	H(4)	114.22(7)	O(1)	H(43)a	144.60(11)

O(1)	,	H(3)	54.89(6)	O(1)	,	H(6)	123.55(8)	C(6)	,	C(2)	124.05(7)	C(6)	,	C(4)	63.41(5)
C(6)	,	O(6)	30.94(5)	C(6)	,	O(61)	78.18(5)	C(6)	,	C(3)	94.66(6)	C(6)	,	O(21)	136.40(6)
C(6)	,	C(21)	140.21(5)	C(6)	,	O(4)a	97.42(6)	C(6)	,	C(4)a	105.33(5)	C(6)	,	H(601)	81.43(11)
C(6)	,	H(1)	171.89(9)	C(6)	,	H(5)	57.50(8)	C(6)	,	H(4)a	113.14(7)	C(6)	,	H(61)	24.18(9)
C(6)	,	H(2)	117.84(8)	C(6)	,	H(63)	45.28(9)	C(6)	,	H(4)	64.19(7)	C(6)	,	H(43)a	81.77(9)
C(6)	,	H(3)	95.81(7)	C(6)	,	H(6)	10.90(7)	C(2)	,	C(4)	60.91(5)	C(2)	,	O(6)	118.34(6)

C(2)	O(61)	149.65(6)	C(2)	C(3)	31.90(4)	C(2)	O(21)	94.28(5)	C(2)	C(21)	75.28(4)
C(2)	O(4)a	84.32(5)	C(2)	C(4)a	98.25(5)	C(2)	H(601)	148.73(12)	C(2)	H(1)	57.68(8)
C(2)	H(5)	94.37(8)	C(2)	H(4)a	102.27(7)	C(2)	H(61)	146.18(11)	C(2)	H(2)	24.41(5)
C(2)	H(63)	128.46(10)	C(2)	H(4)	62.96(6)	C(2)	H(43)a	91.34(10)	C(2)	H(3)	41.44(5)
C(2)	H(6)	114.70(8)	C(4)	O(6)	70.04(6)	C(4)	O(61)	132.51(6)	C(4)	C(3)	32.04(4)
C(4)	O(21)	143.51(6)	C(4)	C(21)	118.41(5)	C(4)	O(4)a	97.05(5)	C(4)	C(4)a	121.06(5)
C(4)	H(601)	136.87(12)	C(4)	H(1)	118.51(9)	C(4)	H(5)	56.15(8)	C(4)	H(4)a	135.36(8)
C(4)	H(61)	85.54(10)	C(4)	H(2)	63.32(7)	C(4)	H(63)	89.53(9)	C(4)	H(4)	23.85(6)
C(4)	H(43)a	88.19(8)	C(4)	H(3)	41.47(5)	C(4)	H(6)	53.79(7)	O(6)	O(61)	91.40(6)
O(6)	C(3)	100.46(6)	O(6)	O(21)	144.82(6)	O(6)	C(21)	166.13(6)	O(6)	O(4)a	66.49(5)
O(6)	C(4)a	76.56(5)	O(6)	H(601)	92.86(11)	O(6)	H(1)	141.06(9)	O(6)	H(5)	87.01(8)
O(6)	H(4)a	87.21(7)	O(6)	H(61)	44.78(8)	O(6)	H(2)	100.63(7)	O(6)	H(63)	20.22(8)
O(6)	H(4)	57.21(6)	O(6)	H(43)a	50.89(9)	O(6)	H(3)	110.99(7)	O(6)	H(6)	37.72(7)
O(61)	C(3)	143.65(6)	O(61)	O(21)	58.93(4)	O(61)	C(21)	74.79(4)	O(61)	O(4)a	115.45(6)
O(61)	C(4)a	94.33(5)	O(61)	H(601)	4.39(11)	O(61)	H(1)	103.53(9)	O(61)	H(5)	80.41(8)
O(61)	H(4)a	83.97(7)	O(61)	H(61)	54.04(10)	O(61)	H(2)	163.33(8)	O(61)	H(63)	81.64(9)
O(61)	H(4)	142.31(8)	O(61)	H(43)a	113.91(10)	O(61)	H(3)	124.93(6)	O(61)	H(6)	84.51(7)
C(3)	O(21)	114.63(5)	C(3)	C(21)	90.26(4)	C(3)	O(4)a	100.75(5)	C(3)	C(4)a	121.77(5)
C(3)	H(601)	146.94(11)	C(3)	H(1)	88.54(8)	C(3)	H(5)	66.22(8)	C(3)	H(4)a	130.44(7)
C(3)	H(61)	114.66(11)	C(3)	H(2)	45.31(6)	C(3)	H(63)	118.36(9)	C(3)	H(4)	44.83(6)
C(3)	H(43)a	99.95(9)	C(3)	H(3)	19.38(5)	C(3)	H(6)	84.37(7)	O(21)	C(21)	25.13(3)
O(21)	O(4)a	107.22(5)	O(21)	C(4)a	86.60(4)	O(21)	H(601)	56.20(10)	O(21)	H(1)	47.26(8)
O(21)	H(5)	104.32(8)	O(21)	H(4)a	72.32(7)	O(21)	H(61)	112.69(10)	O(21)	H(2)	105.62(7)
O(21)	H(63)	126.52(9)	O(21)	H(4)	157.20(7)	O(21)	H(43)a	120.84(8)	O(21)	H(3)	102.10(6)
O(21)	H(6)	139.93(7)	C(21)	O(4)a	120.40(5)	C(21)	C(4)a	105.32(5)	C(21)	H(601)	73.47(11)
C(21)	H(1)	47.02(7)	C(21)	H(5)	89.33(8)	C(21)	H(4)a	92.54(7)	C(21)	H(61)	122.45(9)
C(21)	H(2)	93.17(6)	C(21)	H(63)	151.36(9)	C(21)	H(4)	134.78(7)	C(21)	H(43)a	136.10(9)
C(21)	H(3)	76.98(5)	C(21)	H(6)	136.62(7)	O(4)a	C(4)a	24.11(4)	O(4)a	H(601)	112.31(11)
O(4)a	H(1)	74.64(8)	O(4)a	H(5)	148.44(9)	O(4)a	H(4)a	38.35(6)	O(4)a	H(61)	105.39(8)
O(4)a	H(2)	60.53(6)	O(4)a	H(63)	56.66(9)	O(4)a	H(4)	73.48(6)	O(4)a	H(43)a	15.78(9)
O(4)a	H(3)	119.59(6)	O(4)a	H(6)	102.86(7)	C(4)a	H(601)	90.64(11)	C(4)a	H(1)	66.74(8)
C(4)a	H(5)	162.66(8)	C(4)a	H(4)a	14.69(6)	C(4)a	H(61)	103.16(9)	C(4)a	H(2)	77.53(6)
C(4)a	H(63)	60.06(8)	C(4)a	H(4)	97.34(6)	C(4)a	H(43)a	34.44(7)	C(4)a	H(3)	138.70(6)
C(4)a	H(6)	114.02(7)	H(601)	H(1)	99.89(13)	H(601)	H(5)	84.63(12)	H(601)	H(4)a	79.91(12)
H(601)	H(61)	57.26(13)	H(601)	H(2)	159.33(13)	H(601)	H(63)	81.80(13)	H(601)	H(4)	145.62(12)
H(601)	H(43)a	111.80(14)	H(601)	H(3)	127.89(12)	H(601)	H(6)	88.17(12)	H(1)	H(5)	130.49(11)
H(1)	H(4)a	59.56(9)	H(1)	H(61)	155.91(13)	H(1)	H(2)	59.96(9)	H(1)	H(63)	126.79(11)
H(1)	H(4)	114.02(10)	H(1)	H(43)a	90.34(11)	H(1)	H(3)	89.68(9)	H(1)	H(6)	171.92(11)
H(5)	H(4)a	163.19(10)	H(5)	H(61)	60.38(11)	H(5)	H(2)	111.46(10)	H(5)	H(63)	102.70(11)
H(5)	H(4)	77.87(9)	H(5)	H(43)a	133.87(11)	H(5)	H(3)	52.94(8)	H(5)	H(6)	49.30(9)
H(4)a	H(61)	105.08(11)	H(4)a	H(2)	85.13(8)	H(4)a	H(63)	68.70(10)	H(4)a	H(4)	111.83(8)
H(4)a	H(43)a	49.04(9)	H(4)a	H(3)	143.57(8)	H(4)a	H(6)	123.10(9)	H(61)	H(2)	141.67(11)
H(61)	H(63)	48.79(11)	H(61)	H(4)	88.37(11)	H(61)	H(43)a	91.75(12)	H(61)	H(3)	110.00(11)
H(61)	H(6)	31.99(11)	H(2)	H(63)	105.99(10)	H(2)	H(4)	54.07(8)	H(2)	H(43)a	66.94(11)
H(2)	H(3)	61.20(7)	H(2)	H(6)	112.05(9)	H(63)	H(4)	73.66(10)	H(63)	H(43)a	43.22(12)
H(63)	H(3)	130.88(10)	H(63)	H(6)	54.53(10)	H(4)	H(43)a	64.40(9)	H(4)	H(3)	60.62(7)
H(4)	H(6)	58.02(8)	H(43)a	H(3)	119.29(10)	H(43)a	H(6)	87.09(10)	H(3)	H(6)	84.91(8)

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==================================================================================================================================
 3.6 Angstrom Coordination Sphere Around Atom I =  O(6)  [ARU = 1555.01]         0.58144  0.54530  0.28620    5.8189  4.7468  2.1641
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 Nr     d(I,J) To  Atom J  Symm_Oper. on Atom J    ARU(J)  Type     Phi     Mu         X        Y        Z         XO      YO      ZO
----------------------------------------------------------------------------------------------------------------------------------
 1    0.956(4) --  H(63)  [                    =         ] Intra -76.87   0.18   0.60150  0.43830  0.28660    6.0362  3.8154  2.1671
 2  1.4168(19) --  C(6)   [                    =         ] Intra 169.24 -32.85   0.45754  0.57083  0.18455    4.6496  4.9691  1.3954

 3  2.4310(18) <<  C(5)   [                    =         ] Intra 178.82   1.62   0.35925  0.55107  0.29529    3.3894  4.7971  2.2328
 4  2.7559(19) <<  O(5)   [                    =         ] Intra-151.63  13.07   0.37719  0.39878  0.36864    3.4568  3.4714  2.7874
 5    2.849(2) .<  O(3)a  [1-x,-1/2+y,1-z      =  2646.01]       -65.48   1.67   0.69199  0.24770  0.29720    7.0008  2.1562  2.2472
 6  2.9922(19) <<  C(4)   [                    =         ] Intra 156.57  23.18   0.37404  0.67095  0.44198    3.2951  5.8406  3.3420
 7  3.2202(19) ..  C(61)c [1-x,1/2+y,-z        =  2655.01]         9.14 -51.41   0.71073  0.58194 -0.04668    7.8020  5.0658 -0.3530
 8  3.3469(18) ..  C(1)b  [1-x,1/2+y,1-z       =  2656.01]        71.81  31.14   0.70039  0.85792  0.51513    6.7132  7.4682  3.8951
 9    3.372(2) ..  O(61)c [1-x,1/2+y,-z        =  2655.01]        46.93 -47.08   0.67356  0.73800 -0.04035    7.3872  6.4243 -0.3051
10    3.373(2) ..  O(4)a  [1-x,-1/2+y,1-z      =  2646.01]       -86.12  53.27   0.65120  0.31410  0.64370    5.9554  2.7342  4.8672
11  3.4133(18) ..  O(21)b [1-x,1/2+y,1-z       =  2656.01]        15.42  61.87   0.78795  0.59445  0.68428    7.3704  5.1747  5.1741
12  3.4673(18) ..  C(11)b [1-x,1/2+y,1-z       =  2656.01]        13.41  21.76   0.89699  0.63110  0.45620    8.9514  5.4937  3.4495
13    3.574(2) ..  O(4)   [                    =         ] Intra 138.55   8.53   0.34880  0.81410  0.35630    3.1699  7.0867  2.6941

14    2.030(4) <<  H(6)   [                    =         ] Intra 132.45 -34.40   0.45310  0.68730  0.13450    4.6884  5.9829  1.0170
15    2.064(4) <<  H(61)  [                    =         ] Intra-159.03 -51.71   0.43720  0.49270  0.07190    4.6245  4.2890  0.5437
16    2.268(3) <<  H(1)b  [1-x,1/2+y,1-z       =  2656.01]        70.77  35.69   0.66530  0.74510  0.46120    6.4258  6.4861  3.4873
17    2.436(3) <<  H(12)b [1-x,1/2+y,1-z       =  2656.01]        13.62  14.53   0.80530  0.60910  0.36700    8.1104  5.3022  2.7750
18    2.505(4) <<  H(62)c [1-x,1/2+y,-z        =  2655.01]        -1.34 -36.60   0.73490  0.53990  0.08870    7.8293  4.6998  0.6707
19    2.539(5) .<  H(43)a [1-x,-1/2+y,1-z      =  2646.01]       -75.09  56.89   0.65930  0.39130  0.56750    6.1758  3.4063  4.2910
20    2.623(3) .<  H(4)   [                    =         ] Intra 146.28  42.77   0.47170  0.66810  0.52180    4.2173  5.8158  3.9455
21    3.206(4) ..  H(33)a [1-x,-1/2+y,1-z      =  2646.01]       -49.47  -3.89   0.76820  0.26600  0.25740    7.8978  2.3155  1.9463
22    3.330(4) ..  H(611)c[1-x,1/2+y,-z        =  2655.01]       -12.96 -67.10   0.63280  0.51190 -0.11950    7.0820  4.4561 -0.9036
23    3.370(3) ..  H(5)   [                    =         ] Intra 177.60  -9.93   0.26380  0.56130  0.20930    2.5020  4.8861  1.5826
24    3.421(4) ..  H(601) [                    =         ] Intra-134.92 -16.16   0.34770  0.27800  0.16030    3.4986  2.4200  1.2121
25    3.527(4) ..  H(23)b [1-x,1/2+y,1-z       =  2656.01]        57.36 -16.54   0.72810  0.87240  0.15340    7.6430  7.5942  1.1599

Angles (Degrees)  At1...V...At2 with Vertex V =  O(6)
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 H(63)  ,  C(6)       110.0(3)     H(63)  ,  C(5)       104.3(2)     H(63)  ,  O(5)        75.1(2)     H(63)  ,  O(3)a       11.5(2)
 H(63)  ,  C(4)       123.1(2)     H(63)  ,  C(61)c      87.7(2)     H(63)  ,  C(1)b      136.8(2)     H(63)  ,  O(61)c     112.4(2)
 H(63)  ,  O(4)a       53.6(2)     H(63)  ,  O(21)b      90.9(2)     H(63)  ,  C(11)b      90.2(2)     H(63)  ,  O(4)       143.7(2)
 H(63)  ,  H(6)       136.2(3)     H(63)  ,  H(61)       85.3(3)     H(63)  ,  H(1)b      133.2(3)     H(63)  ,  H(12)b      90.4(2)
 H(63)  ,  H(62)c      78.5(2)     H(63)  ,  H(43)a      56.7(3)     H(63)  ,  H(4)       122.2(3)     H(63)  ,  H(33)a      27.7(2)
 H(63)  ,  H(611)c     80.3(2)     H(63)  ,  H(5)       105.3(2)     H(63)  ,  H(601)      59.5(2)     H(63)  ,  H(23)b     132.0(2)
 C(6)   ,  C(5)       35.64(6)     C(6)   ,  O(5)       59.20(8)     C(6)   ,  O(3)a    120.06(11)     C(6)   ,  C(4)       57.32(7)
 C(6)   ,  C(61)c     93.94(8)     C(6)   ,  C(1)b    111.93(10)     C(6)   ,  O(61)c     84.75(9)     C(6)   ,  O(4)a    124.18(10)
 C(6)   ,  O(21)b   146.50(10)     C(6)   ,  C(11)b   155.91(11)     C(6)   ,  O(4)       50.66(8)     C(6)   ,  H(6)      30.51(12)
 C(6)   ,  H(61)     29.72(12)     C(6)   ,  H(1)b    114.65(13)     C(6)   ,  H(12)b   151.25(14)     C(6)   ,  H(62)c   109.99(12)
 C(6)   ,  H(43)a   130.78(18)     C(6)   ,  H(4)       78.50(9)     C(6)   ,  H(33)a   128.11(12)     C(6)   ,  H(611)c   80.04(10)
 C(6)   ,  H(5)       24.18(7)     C(6)   ,  H(601)    52.84(10)     C(6)   ,  H(23)b    98.38(11)     C(5)   ,  O(5)       31.41(5)
 C(5)   ,  O(3)a     115.63(8)     C(5)   ,  C(4)       30.50(4)     C(5)   ,  C(61)c    129.46(6)     C(5)   ,  C(1)b     103.63(6)
 C(5)   ,  O(61)c    118.37(7)     C(5)   ,  O(4)a      91.73(6)     C(5)   ,  O(21)b    115.26(6)     C(5)   ,  C(11)b    152.61(7)
 C(5)   ,  O(4)       40.67(5)     C(5)   ,  H(6)      56.42(10)     C(5)   ,  H(61)     56.53(10)     C(5)   ,  H(1)b     103.59(9)
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C(5)	, H(12)b	158.19(10)	C(5)	, H(62)c	145.02(10)	C(5)	, H(43)a	97.34(16)	C(5)	, H(4)	50.37(6)
C(5)	, H(33)a	131.73(9)	C(5)	, H(611)c	114.01(8)	C(5)	, H(5)	11.62(5)	C(5)	, H(601)	49.01(7)
C(5)	, H(23)b	120.54(9)	O(5)	, O(3)a	85.88(6)	O(5)	, C(4)	50.00(4)	O(5)	, C(61)c	138.63(7)
O(5)	, C(1)b	119.23(6)	O(5)	, O(61)c	142.61(6)	O(5)	, O(4)a	64.99(5)	O(5)	, O(21)b	104.37(5)
O(5)	, C(11)b	142.20(6)	O(5)	, O(4)	68.54(5)	O(5)	, H(6)	86.12(11)	O(5)	, H(61)	65.10(11)
O(5)	, H(1)b	116.89(9)	O(5)	, H(12)b	148.78(9)	O(5)	, H(62)c	144.50(11)	O(5)	, H(43)a	71.74(15)

O(5) , H(4)	60.77(7)	O(5) , H(33)a	102.72(9)	O(5) , H(611)c	119.54(8)	O(5) , H(5)	38.24(5)
O(5) , H(601)	33.58(5)	O(5) , H(23)b	151.78(8)	O(3)a , C(4)	132.13(7)	O(3)a , C(61)c	81.80(6)
O(3)a , C(1)b	127.84(6)	O(3)a , O(61)c	106.31(6)	O(3)a , O(4)a	54.35(5)	O(3)a , O(21)b	84.24(5)
O(3)a , C(11)b	79.06(5)	O(3)a , O(4)	153.97(7)	O(3)a , H(6)	143.25(12)	O(3)a , H(61)	93.51(14)
O(3)a , H(1)b	124.70(9)	O(3)a , H(12)b	79.03(10)	O(3)a , H(62)c	70.57(9)	O(3)a , H(43)a	55.75(11)
O(3)a , H(4)	127.16(9)	O(3)a , H(33)a	16.94(7)	O(3)a , H(611)c	77.89(8)	O(3)a , H(5)	116.80(7)
O(3)a , H(601)	70.79(7)	O(3)a , H(23)b	121.86(8)	C(4) , C(61)c	142.27(7)	C(4) , C(1)b	74.01(5)
C(4) , O(61)c	119.91(6)	C(4) , O(4)a	86.37(5)	C(4) , O(21)b	89.45(5)	C(4) , C(11)b	122.50(6)
C(4) , O(4)	22.65(4)	C(4) , H(6)	61.98(10)	C(4) , H(61)	84.38(11)	C(4) , H(1)b	73.48(8)
C(4) , H(12)b	127.69(9)	C(4) , H(62)c	156.71(11)	C(4) , H(43)a	88.96(14)	C(4) , H(4)	21.37(5)
C(4) , H(33)a	148.30(9)	C(4) , H(611)c	135.60(8)	C(4) , H(5)	38.99(5)	C(4) , H(601)	77.65(7)
C(4) , H(23)b	104.66(8)	C(61)c , C(1)b	99.16(5)	C(61)c , O(61)c	24.76(4)	C(61)c , O(4)a	131.35(6)
C(61)c , O(21)b	113.39(5)	C(61)c , C(11)b	73.27(4)	C(61)c , O(4)	120.50(6)	C(61)c , H(6)	80.85(10)
C(61)c , H(61)	76.39(10)	C(61)c , H(1)b	102.43(8)	C(61)c , H(12)b	66.05(7)	C(61)c , H(62)c	16.58(8)
C(61)c , H(43)a	128.35(15)	C(61)c , H(4)	150.05(9)	C(61)c , H(33)a	67.84(7)	C(61)c , H(611)c	19.10(6)
C(61)c , H(5)	117.85(6)	C(61)c , H(601)	105.52(6)	C(61)c , H(23)b	51.62(6)	C(1)b , O(61)c	81.37(5)
C(1)b , O(4)a	93.43(5)	C(1)b , O(21)b	47.20(3)	C(1)b , C(11)b	52.54(3)	C(1)b , O(4)	65.73(4)
C(1)b , H(6)	86.90(11)	C(1)b , H(61)	137.81(14)	C(1)b , H(1)b	4.63(6)	C(1)b , H(12)b	55.49(8)
C(1)b , H(62)c	96.27(9)	C(1)b , H(43)a	87.62(10)	C(1)b , H(4)	58.71(6)	C(1)b , H(33)a	118.58(7)
C(1)b , H(611)c	116.49(8)	C(1)b , H(5)	108.58(6)	C(1)b , H(601)	151.42(7)	C(1)b , H(23)b	49.66(5)
O(61)c , O(4)a	149.87(6)	O(61)c , O(21)b	111.84(5)	O(61)c , C(11)b	75.17(4)	O(61)c , O(4)	97.33(6)
O(61)c , H(6)	62.77(10)	O(61)c , H(61)	78.74(11)	O(61)c , H(1)b	85.49(8)	O(61)c , H(12)b	68.45(7)
O(61)c , H(62)c	36.82(9)	O(61)c , H(43)a	144.15(16)	O(61)c , H(4)	125.35(9)	O(61)c , H(33)a	91.49(7)
O(61)c , H(611)c	36.15(7)	O(61)c , H(5)	108.11(6)	O(61)c , H(601)	116.75(6)	O(61)c , H(23)b	31.73(5)
O(4)a , O(21)b	49.43(4)	O(4)a , C(11)b	78.16(5)	O(4)a , O(4)	107.57(6)	O(4)a , H(6)	147.00(12)
O(4)a , H(61)	121.34(13)	O(4)a , H(1)b	88.81(8)	O(4)a , H(12)b	84.09(9)	O(4)a , H(62)c	115.73(10)
O(4)a , H(43)a	7.26(14)	O(4)a , H(4)	73.95(7)	O(4)a , H(33)a	64.90(7)	O(4)a , H(611)c	132.13(9)
O(4)a , H(5)	101.70(7)	O(4)a , H(601)	81.06(7)	O(4)a , H(23)b	133.54(7)	O(21)b , C(11)b	40.13(3)
O(21)b , O(4)	97.13(5)	O(21)b , H(6)	132.46(12)	O(21)b , H(61)	169.41(12)	O(21)b , H(1)b	42.93(7)
O(21)b , H(12)b	47.36(6)	O(21)b , H(62)c	99.40(9)	O(21)b , H(43)a	42.58(11)	O(21)b , H(4)	68.13(6)
O(21)b , H(33)a	81.97(7)	O(21)b , H(611)c	130.61(8)	O(21)b , H(5)	126.46(6)	O(21)b , H(601)	129.71(7)
O(21)b , H(23)b	85.11(6)	C(11)b , O(4)	118.27(6)	C(11)b , H(6)	125.55(12)	C(11)b , H(61)	149.48(11)
C(11)b , H(1)b	51.45(7)	C(11)b , H(12)b	7.24(6)	C(11)b , H(62)c	60.00(8)	C(11)b , H(43)a	71.11(15)
C(11)b , H(4)	102.24(7)	C(11)b , H(33)a	66.59(7)	C(11)b , H(611)c	91.01(7)	C(11)b , H(5)	160.76(7)
C(11)b , H(601)	149.59(8)	C(11)b , H(23)b	57.62(6)	O(4) , H(6)	43.32(10)	O(4) , H(61)	80.37(12)
O(4) , H(1)b	67.03(8)	O(4) , H(12)b	120.72(10)	O(4) , H(62)c	134.08(10)	O(4) , H(43)a	109.00(14)
O(4) , H(4)	34.91(6)	O(4) , H(33)a	170.79(8)	O(4) , H(611)c	118.35(8)	O(4) , H(5)	43.04(6)
O(4) , H(601)	89.07(7)	O(4) , H(23)b	84.09(7)	H(6) , H(61)	50.91(16)	H(6) , H(1)b	90.67(13)
H(6) , H(12)b	121.79(14)	H(6) , H(62)c	96.98(13)	H(6) , H(43)a	150.80(18)	H(6) , H(4)	78.21(11)
H(6) , H(33)a	141.66(12)	H(6) , H(611)c	75.16(12)	H(6) , H(5)	47.88(11)	H(6) , H(601)	83.06(12)
H(6) , H(23)b	68.63(12)	H(61) , H(1)b	141.52(16)	H(61) , H(12)b	142.35(13)	H(61) , H(62)c	89.56(13)
H(61) , H(43)a	128.44(18)	H(61) , H(4)	105.67(12)	H(61) , H(33)a	98.84(14)	H(61) , H(611)c	58.47(11)
H(61) , H(5)	45.92(11)	H(61) , H(601)	40.39(12)	H(61) , H(23)b	104.76(13)	H(1)b , H(12)b	55.05(10)
H(1)b , H(62)c	98.48(11)	H(1)b , H(43)a	83.02(12)	H(1)b , H(4)	56.95(9)	H(1)b , H(33)a	116.59(10)
H(1)b , H(611)c	120.19(10)	H(1)b , H(5)	109.41(9)	H(1)b , H(601)	149.92(10)	H(1)b , H(23)b	53.75(8)
H(12)b , H(62)c	53.04(10)	H(12)b , H(43)a	77.18(16)	H(12)b , H(4)	108.13(10)	H(12)b , H(33)a	65.16(11)
H(12)b , H(611)c	83.92(9)	H(12)b , H(5)	163.68(11)	H(12)b , H(601)	149.65(12)	H(12)b , H(23)b	53.19(10)
H(62)c , H(43)a	112.13(17)	H(62)c , H(4)	154.50(12)	H(62)c , H(33)a	54.89(10)	H(62)c , H(611)c	31.21(10)
H(62)c , H(5)	133.46(10)	H(62)c , H(601)	111.45(10)	H(62)c , H(23)b	55.28(10)	H(43)a , H(4)	74.46(14)

H(43)a ,	H(33)a	64.24(14)	H(43)a ,	H(611)c	132.23(14)	H(43)a ,	H(5)	107.74(16)	H(43)a ,	H(601)	88.24(13)
H(43)a ,	H(23)b	126.29(14)	H(4) ,	H(33)a	138.68(10)	H(4) ,	H(611)c	153.21(10)	H(4) ,	H(5)	59.96(7)
H(4) ,	H(601)	92.98(8)	H(4) ,	H(23)b	100.37(9)	H(33)a ,	H(611)c	68.00(9)	H(33)a ,	H(5)	131.13(9)
H(33)a ,	H(601)	84.56(9)	H(33)a ,	H(23)b	104.92(9)	H(611)c,	H(5)	102.59(8)	H(611)c,	H(601)	86.65(8)
H(611)c,	H(23)b	67.18(8)	H(5) ,	H(601)	46.58(7)	H(5) ,	H(23)b	115.24(8)	H(601) ,	H(23)b	145.14(8)

3.6 Angstrom Coordination Sphere Around Atom I = O(11) [ARU = 1555.01]   0.03017 0.23550 0.62119   -0.7519 2.0500 4.6970

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.974(3)	--	H(101)	[	=]	Intra	55.54	14.84	0.08450	0.32470	0.65420	-0.2191	2.8265	4.9466
2	1.4232(19)	--	C(11)	[	=]	Intra	-44.47	-24.28	0.10301	0.13110	0.54380	0.1739	1.1412	4.1118
3	2.4324(15)	<<	C(21)	[	=]	Intra	-14.32	-51.64	0.12446	0.19262	0.36895	0.7108	1.6768	2.7897
4	2.7157(18)	<<	O(41)a	[x,y,1+z	= 1556.01]		-131.45	53.79	-0.02123	0.09734	0.91096	-1.8139	0.8473	6.8881
5	2.7715(17)	<<	O(1)	[	=]	Intra	26.51	-38.77	0.17143	0.34630	0.39165	1.1816	3.0145	2.9614
6	2.781(2)	<<	O(2)	[	=]	Intra	41.82	20.11	0.22954	0.43550	0.74766	1.1941	3.7910	5.6533
7	3.1305(15)	.<	C(31)	[	=]	Intra	-40.48	-78.95	0.00718	0.19075	0.21485	-0.2954	1.6605	1.6245
8	3.2561(18)	..	O(31)	[	=]	Intra	119.42	-75.38	-0.07367	0.31776	0.20452	-1.1558	2.7661	1.5464
9	3.3542(15)	..	C(41)a	[x,y,1+z	= 1556.01]		-122.17	77.79	0.06478	0.16653	1.05476	-1.1295	1.4496	7.9754
10	3.4941(16)	..	C(1)	[	=]	Intra	18.61	-17.16	0.29961	0.35792	0.48487	2.4120	3.1157	3.6663
11	3.5153(17)	..	C(3)b	[-x,-1/2+y,1-z	= 2546.01]		-164.53	-23.54	-0.28545	0.13673	0.43553	-3.8579	1.1902	3.2932
12	1.760(3)	<<	H(401)a	[x,y,1+z	= 1556.01]		-139.30	51.71	-0.01670	0.15380	0.80390	-1.5786	1.3388	6.0785
13	2.044(3)	<<	H(11)	[	=]	Intra	-77.53	-21.62	0.05200	0.02240	0.52160	-0.3417	0.1950	3.9440
14	2.083(3)	<<	H(12)	[	=]	Intra	-31.91	2.46	0.19470	0.10910	0.63300	1.0149	0.9497	4.7863
15	2.455(3)	<<	H(3)b	[-x,-1/2+y,1-z	= 2546.01]		-159.99	-19.97	-0.18710	0.14480	0.51030	-2.9194	1.2605	3.8585
16	2.796(3)	..	H(11)c	[-x,1/2+y,1-z	= 2556.01]		104.47	-22.71	-0.05200	0.52240	0.47840	-1.3964	4.5475	3.6173
17	3.004(3)	..	H(41)a	[x,y,1+z	= 1556.01]		81.25	82.98	0.09840	0.27720	1.01550	-0.6960	2.4130	7.6785
18	3.052(3)	..	H(23)	[	=]	Intra	28.08	33.94	0.27190	0.37240	0.84660	1.4823	3.2417	6.4014
19	3.235(3)	..	H(31)	[	=]	Intra	-98.17	-66.43	-0.04950	0.08840	0.22900	-0.9357	0.7695	1.7315
20	3.248(3)	..	H(301)b	[-x,-1/2+y,1-z	= 2546.01]		-96.89	28.16	0.03100	-0.09110	0.82390	-1.0952	-0.7930	6.2298
21	3.275(3)	..	H(31)c	[-x,1/2+y,1-z	= 2556.01]		90.94	20.24	0.04950	0.58840	0.77100	-0.8023	5.1220	5.8298
22	3.450(4)	..	H(62)a	[x,y,1+z	= 1556.01]		-39.74	39.48	0.26510	0.03990	0.91130	1.2960	0.3473	6.8906
23	3.508(3)	..	H(1)	[	=]	Intra	1.39	-10.23	0.33470	0.24510	0.53880	2.6995	2.1336	4.0740
24	3.541(3)	..	H(33)b	[-x,-1/2+y,1-z	= 2546.01]		173.16	-50.98	-0.23180	0.26600	0.25740	-2.9655	2.3155	1.9463
25	3.588(3)	..	H(51)c	[-x,1/2+y,1-z	= 2556.01]		143.20	34.03	-0.14650	0.44010	0.88670	-3.1326	3.8311	6.7046

Angles (Degrees) At1...V...At2 with Vertex V = O(11)

H(101) ,	C(11)	105.0(2)	H(101) ,	C(21)	89.67(18)	H(101) ,	O(41)a	111.11(16)	H(101) ,	O(1)	60.10(17)
H(101) ,	O(2)	14.10(18)	H(101) ,	C(31)	105.72(17)	H(101) ,	O(31)	98.07(16)	H(101) ,	C(41)a	87.35(16)
H(101) ,	C(1)	48.49(18)	H(101) ,	C(3)b	141.3(2)	H(101) ,	H(401)a	112.20(19)	H(101) ,	H(11)	135.1(2)
H(101) ,	H(12)	86.9(2)	H(101) ,	H(3)b	145.8(2)	H(101) ,	H(11)c	60.86(19)	H(101) ,	H(41)a	68.85(16)
H(101) ,	H(23)	31.29(18)	H(101) ,	H(31)	125.55(17)	H(101) ,	H(301)b	129.39(18)	H(101) ,	H(31)c	34.1(2)
H(101) ,	H(62)a	84.60(19)	H(101) ,	H(1)	59.2(2)	H(101) ,	H(33)b	118.76(19)	H(101) ,	H(51)c	79.9(2)
C(11) ,	C(21)	35.75(6)	C(11) ,	O(41)a	107.66(10)	C(11) ,	O(1)	60.72(7)	C(11) ,	O(2)	94.93(8)
C(11) ,	C(31)	54.70(6)	C(11) ,	O(31)	79.82(7)	C(11) ,	C(41)a	111.15(8)	C(11) ,	C(1)	58.96(7)
C(11) ,	C(3)b	104.74(8)	C(11) ,	H(401)a	111.73(14)	C(11) ,	H(11)	30.49(11)	C(11) ,	H(12)	29.39(8)
C(11) ,	H(3)b	103.21(11)	C(11) ,	H(11)c	124.16(11)	C(11) ,	H(41)a	118.24(9)	C(11) ,	H(23)	90.16(10)
C(11) ,	H(31)	53.65(7)	C(11) ,	H(301)b	72.77(9)	C(11) ,	H(31)c	138.70(10)	C(11) ,	H(62)a	63.91(8)
C(11) ,	H(1)	45.75(8)	C(11) ,	H(33)b	97.77(9)	C(11) ,	H(51)c	168.18(10)	C(21) ,	O(41)a	143.11(8)
C(21) ,	O(1)	31.00(4)	C(21) ,	O(2)	86.84(6)	C(21) ,	C(31)	28.79(3)	C(21) ,	O(31)	49.43(4)
C(21) ,	C(41)a	143.77(6)	C(21) ,	C(1)	43.19(4)	C(21) ,	C(3)b	100.41(5)	C(21) ,	H(401)a	146.71(13)
C(21) ,	H(11)	56.71(10)	C(21) ,	H(12)	56.12(8)	C(21) ,	H(3)b	102.35(7)	C(21) ,	H(11)c	88.45(8)

C(21) ,	H(41)a	141.78(7)	C(21) ,	H(23)	93.30(7)	C(21) ,	H(31)	41.82(5)	C(21) ,	H(301)b	107.41(8)
C(21) ,	H(31)c	115.12(7)	C(21) ,	H(62)a	93.78(7)	C(21) ,	H(1)	43.35(5)	C(21) ,	H(33)b	77.19(6)
C(21) ,	H(51)c	156.07(8)	O(41)a ,	O(1)	158.78(7)	O(41)a ,	O(2)	105.87(6)	O(41)a ,	C(31)	142.54(7)
O(41)a ,	O(31)	146.05(6)	O(41)a ,	C(41)a	24.24(4)	O(41)a ,	C(1)	136.65(5)	O(41)a ,	C(3)b	82.44(5)
O(41)a ,	H(401)a	5.18(11)	O(41)a ,	H(11)	88.50(11)	O(41)a ,	H(12)	93.62(9)	O(41)a ,	H(3)b	77.75(7)
O(41)a ,	H(11)c	128.09(9)	O(41)a ,	H(41)a	42.27(6)	O(41)a ,	H(23)	90.49(7)	O(41)a ,	H(31)	122.82(8)

O(41)a	H(301)b	35.93(6)	O(41)a	H(31)c	97.49(7)	O(41)a	H(62)a	60.04(7)	O(41)a	H(1)	122.59(7)
O(41)a	H(33)b	114.55(7)	O(41)a	H(51)c	60.58(6)	O(1)	O(2)	60.61(5)	O(1)	C(31)	47.70(4)
O(1)	O(31)	53.42(4)	O(1)	C(41)a	138.84(5)	O(1)	C(1)	22.69(3)	O(1)	C(3)b	116.84(5)
O(1)	H(401)a	163.71(12)	O(1)	H(11)	86.85(10)	O(1)	H(12)	67.60(9)	O(1)	H(3)b	120.94(7)
O(1)	H(11)c	66.93(8)	O(1)	H(41)a	124.51(7)	O(1)	H(23)	72.73(6)	O(1)	H(31)	66.63(5)
O(1)	H(301)b	132.37(7)	O(1)	H(31)c	84.31(6)	O(1)	H(62)a	98.96(7)	O(1)	H(1)	36.31(5)
O(1)	H(33)b	85.61(6)	O(1)	H(51)c	129.84(8)	O(2)	C(31)	108.26(5)	O(2)	O(31)	106.37(6)
O(2)	C(41)a	81.65(5)	O(2)	C(1)	43.68(4)	O(2)	C(3)b	155.34(7)	O(2)	H(401)a	108.17(11)
O(2)	H(11)	123.68(11)	O(2)	H(12)	73.89(10)	O(2)	H(3)b	159.53(10)	O(2)	H(11)c	74.63(8)
O(2)	H(41)a	64.53(6)	O(2)	H(23)	18.43(7)	O(2)	H(31)	127.07(7)	O(2)	H(301)b	117.37(7)
O(2)	H(31)c	45.93(6)	O(2)	H(62)a	71.03(7)	O(2)	H(1)	50.03(5)	O(2)	H(33)b	131.13(8)
O(2)	H(51)c	87.77(7)	C(31)	O(31)	25.28(3)	C(31)	C(41)a	162.44(7)	C(31)	C(1)	67.44(3)
C(31)	C(3)b	72.93(4)	C(31)	H(401)a	142.05(12)	C(31)	H(11)	59.74(9)	C(31)	H(12)	81.53(8)
C(31)	H(3)b	75.73(6)	C(31)	H(11)c	76.45(7)	C(31)	H(41)a	170.55(7)	C(31)	H(23)	119.33(7)
C(31)	H(31)	19.86(5)	C(31)	H(301)b	111.69(7)	C(31)	H(31)c	117.29(7)	C(31)	H(62)a	118.43(7)
C(31)	H(1)	71.65(5)	C(31)	H(33)b	48.55(6)	C(31)	H(51)c	135.05(6)	O(31)	C(41)a	166.20(5)
O(31)	C(1)	76.10(4)	O(31)	C(3)b	63.75(4)	O(31)	H(401)a	142.19(12)	O(31)	H(11)	82.41(10)
O(31)	H(12)	105.24(8)	O(31)	H(3)b	68.33(7)	O(31)	H(11)c	53.23(7)	O(31)	H(41)a	159.40(8)
O(31)	H(23)	123.04(7)	O(31)	H(31)	36.21(5)	O(31)	H(301)b	129.49(7)	O(31)	H(31)c	97.27(6)
O(31)	H(62)a	142.87(7)	O(31)	H(1)	86.84(5)	O(31)	H(33)b	32.25(6)	O(31)	H(51)c	110.49(6)
C(41)a	C(1)	116.41(4)	C(41)a	C(3)b	104.30(4)	C(41)a	H(401)a	26.83(10)	C(41)a	H(11)	102.72(10)
C(41)a	H(12)	87.65(8)	C(41)a	H(3)b	100.19(7)	C(41)a	H(11)c	120.75(8)	C(41)a	H(41)a	18.86(5)
C(41)a	H(23)	66.83(6)	C(41)a	H(31)	144.95(8)	C(41)a	H(301)b	50.97(5)	C(41)a	H(31)c	80.10(6)
C(41)a	H(62)a	49.99(6)	C(41)a	H(1)	106.77(5)	C(41)a	H(33)b	134.62(7)	C(41)a	H(51)c	57.81(5)
C(1)	C(3)b	139.19(4)	C(1)	H(401)a	141.27(12)	C(1)	H(11)	89.22(10)	C(1)	H(12)	53.54(9)
C(1)	H(3)b	142.84(7)	C(1)	H(11)c	79.77(8)	C(1)	H(41)a	103.83(6)	C(1)	H(23)	51.89(6)
C(1)	H(31)	84.36(5)	C(1)	H(301)b	120.12(6)	C(1)	H(31)c	80.20(5)	C(1)	H(62)a	78.50(6)
C(1)	H(1)	18.10(4)	C(1)	H(33)b	108.30(6)	C(1)	H(51)c	127.92(7)	C(3)b	H(401)a	78.44(11)
C(3)b	H(11)	78.94(10)	C(3)b	H(12)	129.59(11)	C(3)b	H(3)b	5.52(6)	C(3)b	H(11)c	81.99(8)
C(3)b	H(41)a	116.25(6)	C(3)b	H(23)	164.85(8)	C(3)b	H(31)	59.13(5)	C(3)b	H(301)b	83.16(6)
C(3)b	H(31)c	110.73(6)	C(3)b	H(62)a	131.12(8)	C(3)b	H(1)	143.53(6)	C(3)b	H(33)b	32.40(6)
C(3)b	H(51)c	76.03(6)	H(401)a	H(11)	90.96(14)	H(401)a	H(12)	98.70(14)	H(401)a	H(3)b	73.94(12)
H(401)a	H(11)c	123.76(13)	H(401)a	H(41)a	43.82(10)	H(401)a	H(23)	93.63(12)	H(401)a	H(31)	122.20(12)
H(401)a	H(301)b	39.31(10)	H(401)a	H(31)c	95.76(11)	H(401)a	H(62)a	65.19(12)	H(401)a	H(1)	127.67(12)
H(401)a	H(33)b	110.27(13)	H(401)a	H(51)c	56.61(11)	H(11)	H(12)	50.67(13)	H(11)	H(3)b	76.08(12)
H(11)	H(11)c	135.62(12)	H(11)	H(41)a	118.14(11)	H(11)	H(23)	114.41(12)	H(11)	H(31)	46.72(10)
H(11)	H(301)b	53.17(10)	H(11)	H(31)c	169.14(12)	H(11)	H(62)a	70.56(11)	H(11)	H(1)	76.04(11)
H(11)	H(33)b	84.68(11)	H(11)	H(51)c	142.19(12)	H(12)	H(3)b	126.42(13)	H(12)	H(11)c	133.14(12)
H(12)	H(41)a	90.32(9)	H(12)	H(23)	63.99(11)	H(12)	H(31)	83.02(9)	H(12)	H(301)b	66.87(10)
H(12)	H(31)c	119.58(11)	H(12)	H(62)a	37.70(9)	H(12)	H(1)	35.50(10)	H(12)	H(33)b	127.09(10)
H(12)	H(51)c	143.23(9)	H(3)b	H(11)c	87.24(10)	H(3)b	H(41)a	113.22(8)	H(3)b	H(23)	164.31(9)
H(3)b	H(31)	60.62(7)	H(3)b	H(301)b	77.66(8)	H(3)b	H(31)c	113.98(9)	H(3)b	H(62)a	125.63(10)
H(3)b	H(1)	144.67(8)	H(3)b	H(33)b	37.50(8)	H(3)b	H(51)c	76.40(8)	H(11)c	H(41)a	106.24(9)
H(11)c	H(23)	92.04(10)	H(11)c	H(31)	89.23(8)	H(11)c	H(301)b	159.99(9)	H(11)c	H(31)c	44.94(8)
H(11)c	H(62)a	145.39(10)	H(11)c	H(1)	97.87(9)	H(11)c	H(33)b	59.27(9)	H(11)c	H(51)c	67.65(8)
H(41)a	H(23)	52.05(7)	H(41)a	H(31)	163.45(9)	H(41)a	H(301)b	68.86(7)	H(41)a	H(31)c	62.84(7)
H(41)a	H(62)a	54.38(7)	H(41)a	H(1)	98.92(7)	H(41)a	H(33)b	140.68(8)	H(41)a	H(51)c	52.91(7)
H(23)	H(31)	135.07(8)	H(23)	H(301)b	98.95(8)	H(23)	H(31)c	56.76(8)	H(23)	H(62)a	53.36(9)
H(23)	H(1)	50.93(7)	H(23)	H(33)b	149.56(10)	H(23)	H(51)c	88.82(8)	H(31)	H(301)b	94.59(8)

H(31)	H(31)c	133.43(8)	H(31)	H(62)a	114.91(8)	H(31)	H(1)	84.41(6)	H(31)	H(33)b	44.12(7)
H(31)	H(51)c	132.20(7)	H(301)b	H(31)c	131.02(7)	H(301)b	H(62)a	47.99(7)	H(301)b	H(1)	102.04(7)
H(301)b	H(33)b	111.48(8)	H(301)b	H(51)c	95.76(7)	H(31)c	H(62)a	104.61(8)	H(31)c	H(1)	93.11(7)
H(31)c	H(33)b	100.88(8)	H(31)c	H(51)c	47.97(6)	H(62)a	H(1)	62.66(7)	H(62)a	H(33)b	154.42(10)
H(62)a	H(51)c	106.44(7)	H(1)	H(33)b	118.38(7)	H(1)	H(51)c	137.77(8)	H(33)b	H(51)c	89.01(8)

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==================================================================================================================================
 3.6 Angstrom Coordination Sphere Around Atom I =  O(21) [ARU = 1555.01]         0.21205  0.09445  0.31572    1.7548  0.8222  2.3873
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 Nr     d(I,J) To  Atom J  Symm_Oper. on Atom J    ARU(J)  Type     Phi     Mu         X         Y         Z         XO      YO      ZO
----------------------------------------------------------------------------------------------------------------------------------
 1  1.4079(16) --  C(21)  [                     =         ] Intra 140.70  16.61   0.12446  0.19262  0.36895    0.7108  1.6768  2.7897
 2  1.4450(14) --  C(51)  [                     =         ] Intra-102.26 -78.22   0.17635  0.06133  0.12864    1.6922  0.5339  0.9727

 3  2.3377(19) <<  O(1)   [                     =         ] Intra 104.65  14.22   0.17143  0.34630  0.39165    1.1816  3.0145  2.9614
 4  2.3426(15) <<  C(31)  [                     =         ] Intra 157.76 -19.00   0.00718  0.19075  0.21485   -0.2954  1.6605  1.6245
 5  2.3612(15) <<  C(11)  [                     =         ] Intra 168.59  46.92   0.10301  0.13110  0.54380    0.1739  1.1412  4.1118
 6  2.3667(14) <<  C(41)  [                     =         ] Intra 151.30 -56.48   0.06478  0.16653  0.05476    0.6086  1.4496  0.4141
 7  2.4201(15) <<  C(61)  [                     =         ] Intra  -4.76 -57.20   0.28927  0.08194  0.04668    3.0613  0.7133  0.3530
 8  2.7070(14) <<  C(1)   [                     =         ] Intra  74.01  28.20   0.29961  0.35792  0.48487    2.4120  3.1157  3.6663
 9    2.838(2) <<  O(4)a  [x,-1+y,z             =  1545.01]       -59.89   6.21   0.34880 -0.18590  0.35630    3.1699 -1.6183  2.6941
10  2.9765(18) .<  O(61)  [                     =         ] Intra  35.98 -44.39   0.32644  0.23800  0.04035    3.4761  2.0718  0.3051
11  3.1741(19) ..  O(5)   [                     =         ] Intra  57.28   7.24   0.37719  0.39878  0.36864    3.4568  3.4714  2.7874
12  3.4133(18) ..  O(6)b  [1-x,-1/2+y,1-z       =  2646.01]       -15.42  61.87   0.41856  0.04530  0.71380    3.3063  0.3943  5.3973
13  3.5664(15) ..  O(41)  [                     =         ] Intra 179.21 -59.11  -0.02123  0.09734 -0.08904   -0.0759  0.8473 -0.6733
14  3.5996(18) ..  O(31)  [                     =         ] Intra 146.26 -13.51  -0.07367  0.31776  0.20452   -1.1558  2.7661  1.5464

15    2.068(3) <<  H(51)  [                     =         ] Intra-105.01 -47.73   0.14650 -0.05990  0.11330    1.3946 -0.5214  0.8567
16    2.310(5) <<  H(43)a [x,-1+y,z             =  1545.01]       -55.96  22.48   0.34070 -0.10870  0.43250    2.9494 -0.9462  3.2703
17    2.336(3) <<  H(1)   [                     =         ] Intra  54.23  46.22   0.33470  0.24510  0.53880    2.6995  2.1336  4.0740
18    2.514(2) <<  H(12)  [                     =         ] Intra 170.22  72.62   0.19470  0.10910  0.63300    1.0149  0.9497  4.7863
19    2.612(4) .<  H(611) [                     =         ] Intra -19.52 -34.61   0.36720  0.01190  0.11950    3.7813  0.1036  0.9036
20    2.641(3) .<  H(601) [                     =         ] Intra  42.50 -26.42   0.34770  0.27800  0.16030    3.4986  2.4200  1.2121
21    2.686(3) .<  H(11)  [                     =         ] Intra-163.34  35.43   0.05200  0.02240  0.52160   -0.3417  0.1950  3.9440
22    2.770(3) ..  H(31)  [                     =         ] Intra-178.88 -13.69  -0.04950  0.08840  0.22900   -0.9357  0.7695  1.7315
23    2.862(3) ..  H(41)  [                     =         ] Intra 114.14 -52.48   0.09840  0.27720  0.01550    1.0420  2.4130  0.1172
24    3.349(3) ..  H(62)  [                     =         ] Intra -20.37 -65.95   0.26510  0.03990 -0.08870    3.0340  0.3473 -0.6707
25    3.444(3) ..  H(4)b  [1-x,-1/2+y,1-z       =  2646.01]        11.49  20.90   0.52830  0.16810  0.47820    4.9080  1.4633  3.6158
26    3.559(4) ..  H(63)b [1-x,-1/2+y,1-z       =  2646.01]       -45.53  57.65   0.39850 -0.06170  0.71340    3.0891 -0.5371  5.3942

Angles (Degrees)  At1...V...At2 with Vertex V =  O(21)
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 C(21)  ,  C(51)     111.64(9)     C(21)  ,  O(1)       34.79(6)     C(21)  ,  C(31)      39.37(5)     C(21)  ,  C(11)       38.07(6)
 C(21)  ,  C(41)      73.64(6)     C(21)  ,  C(61)     131.91(8)     C(21)  ,  C(1)       62.01(7)     C(21)  ,  O(4)a      149.41(9)
 C(21)  ,  O(61)     111.96(8)     C(21)  ,  O(5)       81.66(8)     C(21)  ,  O(6)b      99.27(6)     C(21)  ,  O(41)       81.97(6)
 C(21)  ,  O(31)      30.62(5)     C(21)  ,  H(51)    118.47(12)     C(21)  ,  H(43)a   137.65(15)     C(21)  ,  H(1)        75.68(8)
 C(21)  ,  H(12)      58.54(8)     C(21)  ,  H(611)   154.76(12)     C(21)  ,  H(601)   104.45(11)     C(21)  ,  H(11)       52.93(8)
 C(21)  ,  H(31)      50.13(7)     C(21)  ,  H(41)      72.82(7)     C(21)  ,  H(62)     129.08(9)     C(21)  ,  H(4)b      117.64(8)
 C(21)  ,  H(63)b    105.56(8)     C(51)  ,  O(1)      114.64(9)     C(51)  ,  C(31)      73.42(6)     C(51)  ,  C(11)      135.47(8)
 C(51)  ,  C(41)      38.35(6)     C(51)  ,  C(61)      36.06(6)     C(51)  ,  C(1)      129.95(9)     C(51)  ,  O(4)a       87.47(8)
 C(51)  ,  O(61)      54.83(7)     C(51)  ,  O(5)      108.25(8)     C(51)  ,  O(6)b     149.09(8)     C(51)  ,  O(41)       30.58(6)
 C(51)  ,  O(31)      81.03(7)     C(51)  ,  H(51)      30.50(9)     C(51)  ,  H(43)a   104.12(14)     C(51)  ,  H(1)       146.76(11)
 C(51)  ,  H(12)    158.69(10)     C(51)  ,  H(611)    54.74(10)     C(51)  ,  H(601)     73.37(8)     C(51)  ,  H(11)      119.14(10)
 C(51)  ,  H(31)      73.88(8)     C(51)  ,  H(41)      47.44(8)     C(51)  ,  H(62)      25.08(7)     C(51)  ,  H(4)b      115.22(8)
 C(51)  ,  H(63)b   140.09(10)     O(1)   ,  C(31)      61.95(5)     O(1)   ,  C(11)      61.95(5)     O(1)   ,  C(41)       80.64(6)
 O(1)   ,  C(61)     112.40(7)     O(1)   ,  C(1)       31.67(4)     O(1)   ,  O(4)a     154.46(6)     O(1)   ,  O(61)       85.40(6)
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O(1) ,	O(5)	46.98(4)	O(1) ,	O(6)b	90.71(5)	O(1) ,	O(41)	94.49(5)	O(1) ,	O(31)	49.66(4)
O(1) ,	H(51)	138.44(10)	O(1) ,	H(43)a	138.68(12)	O(1) ,	H(1)	52.80(7)	O(1) ,	H(12)	69.26(9)
O(1) ,	H(611)	125.99(10)	O(1) ,	H(601)	72.77(8)	O(1) ,	H(11)	83.41(7)	O(1) ,	H(31)	80.66(7)
O(1) ,	H(41)	67.20(6)	O(1) ,	H(62)	116.81(8)	O(1) ,	H(4)b	87.84(6)	O(1) ,	H(63)b	104.04(7)
C(31) ,	C(11)	66.64(4)	C(31) ,	C(41)	37.80(4)	C(31) ,	C(61)	102.41(5)	C(31) ,	C(1)	93.62(6)
C(31) ,	O(4)a	141.20(7)	C(31) ,	O(61)	97.36(5)	C(31) ,	O(5)	102.22(6)	C(31) ,	O(6)b	136.87(5)

C(31)	H(1)	112.84(8)	C(31)	H(12)	92.00(7)	C(31)	H(611)	126.33(9)	C(31)	H(601)	102.50(9)
C(31)	O(41)	43.01(4)	C(31)	O(31)	12.32(4)	C(31)	H(51)	80.74(10)	C(31)	H(43)a	148.34(16)
C(31)	H(11)	65.74(7)	C(31)	H(31)	23.01(6)	C(31)	H(41)	47.54(5)	C(31)	H(62)	95.03(7)
C(31)	H(4)b	148.29(8)	C(31)	H(63)b	137.71(7)	C(11)	C(41)	104.41(6)	C(11)	C(61)	168.95(7)
C(11)	C(1)	72.72(5)	C(11)	O(4)a	111.78(6)	C(11)	O(61)	147.29(7)	C(11)	O(5)	98.87(6)
C(11)	O(6)b	71.17(4)	C(11)	O(41)	106.39(5)	C(11)	O(31)	63.66(4)	C(11)	H(51)	120.77(11)
C(11)	H(43)a	99.82(14)	C(11)	H(1)	70.58(7)	C(11)	H(12)	25.71(6)	C(11)	H(611)	166.26(10)
C(11)	H(601)	133.26(9)	C(11)	H(11)	23.86(7)	C(11)	H(31)	61.65(6)	C(11)	H(41)	109.72(7)
C(11)	H(62)	160.38(8)	C(11)	H(4)b	109.10(6)	C(11)	H(63)b	71.67(7)	C(41)	C(61)	64.70(4)
C(41)	C(1)	106.67(6)	C(41)	O(4)a	124.03(6)	C(41)	O(61)	65.52(4)	C(41)	O(5)	98.25(6)
C(41)	O(6)b	171.35(7)	C(41)	O(41)	14.99(4)	C(41)	O(31)	43.15(4)	C(41)	H(51)	58.05(8)
C(41)	H(43)a	140.56(13)	C(41)	H(1)	130.47(9)	C(41)	H(12)	129.77(8)	C(41)	H(611)	88.57(9)
C(41)	H(601)	77.78(7)	C(41)	H(11)	99.62(8)	C(41)	H(31)	48.48(6)	C(41)	H(41)	21.68(6)
C(41)	H(62)	57.40(7)	C(41)	H(4)b	133.75(7)	C(41)	H(63)b	170.80(8)	C(61)	C(1)	107.71(6)
C(61)	O(4)a	77.47(6)	C(61)	O(61)	28.20(5)	C(61)	O(5)	81.61(5)	C(61)	O(6)b	119.36(5)
C(61)	O(41)	63.65(4)	C(61)	O(31)	105.33(5)	C(61)	H(51)	56.14(9)	C(61)	H(43)a	90.44(14)
C(61)	H(1)	114.45(8)	C(61)	H(12)	164.45(8)	C(61)	H(611)	24.69(9)	C(61)	H(601)	45.31(7)
C(61)	H(11)	153.92(9)	C(61)	H(31)	108.94(7)	C(61)	H(41)	59.52(6)	C(61)	H(62)	11.41(6)
C(61)	H(4)b	79.28(5)	C(61)	H(63)b	119.38(7)	C(1)	O(4)a	123.81(6)	C(1)	O(61)	80.47(5)
C(1)	O(5)	26.25(3)	C(1)	O(6)b	65.11(4)	C(1)	O(41)	121.61(5)	C(1)	O(31)	81.32(4)
C(1)	H(51)	160.45(9)	C(1)	H(43)a	110.03(12)	C(1)	H(1)	23.80(7)	C(1)	H(12)	65.01(8)
C(1)	H(611)	108.24(9)	C(1)	H(601)	62.44(7)	C(1)	H(11)	96.52(7)	C(1)	H(31)	111.33(7)
C(1)	H(41)	87.95(7)	C(1)	H(62)	117.31(7)	C(1)	H(4)b	56.74(5)	C(1)	H(63)b	80.41(6)
O(4)a	O(61)	98.53(6)	O(4)a	O(5)	115.90(6)	O(4)a	O(6)b	64.54(5)	O(4)a	O(41)	110.78(6)
O(4)a	O(31)	153.24(6)	O(4)a	H(51)	66.93(9)	O(4)a	H(43)a	16.71(11)	O(4)a	H(1)	101.72(8)
O(4)a	H(12)	95.00(9)	O(4)a	H(611)	55.81(9)	O(4)a	H(601)	103.84(9)	O(4)a	H(11)	97.22(8)
O(4)a	H(31)	119.58(8)	O(4)a	H(41)	133.47(7)	O(4)a	H(62)	77.66(7)	O(4)a	H(4)b	70.43(6)
O(4)a	H(63)b	52.65(7)	O(61)	O(5)	55.09(4)	O(61)	O(6)b	113.99(5)	O(61)	O(41)	72.16(4)
O(61)	O(31)	94.44(5)	O(61)	H(51)	81.71(9)	O(61)	H(43)a	106.85(15)	O(61)	H(1)	92.04(8)
O(61)	H(12)	144.74(9)	O(61)	H(611)	43.08(9)	O(61)	H(601)	18.72(6)	O(61)	H(11)	162.74(8)
O(61)	H(31)	113.84(7)	O(61)	H(41)	49.90(6)	O(61)	H(62)	36.85(7)	O(61)	H(4)b	69.02(5)
O(61)	H(63)b	122.31(7)	O(5)	O(6)b	75.51(4)	O(5)	O(41)	112.18(5)	O(5)	O(31)	90.70(5)
O(5)	H(51)	136.79(9)	O(5)	H(43)a	108.27(14)	O(5)	H(1)	39.07(7)	O(5)	H(12)	89.72(8)
O(5)	H(611)	83.41(9)	O(5)	H(601)	36.59(7)	O(5)	H(11)	122.71(7)	O(5)	H(31)	124.51(7)
O(5)	H(41)	76.68(6)	O(5)	H(62)	91.64(7)	O(5)	H(4)b	46.27(5)	O(5)	H(63)b	90.64(7)
O(6)b	O(41)	172.31(6)	O(6)b	O(31)	129.88(5)	O(6)b	H(51)	130.57(10)	O(6)b	H(43)a	48.07(11)
O(6)b	H(1)	41.39(7)	O(6)b	H(12)	45.46(6)	O(6)b	H(611)	96.53(9)	O(6)b	H(601)	99.68(7)
O(6)b	H(11)	79.30(8)	O(6)b	H(31)	130.39(6)	O(6)b	H(41)	151.92(7)	O(6)b	H(62)	127.87(7)
O(6)b	H(4)b	44.98(5)	O(6)b	H(63)b	15.58(6)	O(41)	O(31)	51.73(3)	O(41)	H(51)	43.95(8)
O(41)	H(43)a	126.80(12)	O(41)	H(1)	145.41(9)	O(41)	H(12)	131.88(7)	O(41)	H(611)	84.99(9)
O(41)	H(601)	87.29(7)	O(41)	H(11)	95.65(8)	O(41)	H(31)	45.44(5)	O(41)	H(41)	35.67(6)
O(41)	H(62)	54.08(6)	O(41)	H(4)b	140.78(5)	O(41)	H(63)b	156.94(8)	O(31)	H(51)	92.13(9)
O(31)	H(43)a	157.08(16)	O(31)	H(1)	101.10(8)	O(31)	H(12)	87.57(7)	O(31)	H(611)	130.03(9)
O(31)	H(601)	95.92(8)	O(31)	H(11)	68.30(7)	O(31)	H(31)	33.85(6)	O(31)	H(41)	46.62(5)
O(31)	H(62)	99.91(7)	O(31)	H(4)b	136.31(6)	O(31)	H(63)b	134.96(7)	H(51)	H(43)a	82.85(14)
H(51)	H(1)	165.80(12)	H(51)	H(12)	133.47(12)	H(51)	H(611)	62.36(12)	H(51)	H(601)	100.30(10)
H(51)	H(11)	98.12(11)	H(51)	H(31)	69.10(11)	H(51)	H(41)	74.38(9)	H(51)	H(62)	45.46(10)
H(51)	H(4)b	122.98(11)	H(51)	H(63)b	116.26(10)	H(43)a	H(1)	86.83(13)	H(43)a	H(12)	79.99(14)
H(43)a	H(611)	66.75(16)	H(43)a	H(601)	106.97(17)	H(43)a	H(11)	90.19(16)	H(43)a	H(31)	125.34(16)

H(43)a ,	H(41)	149.05(14)	H(43)a ,	H(62)	92.46(14)	H(43)a ,	H(4)b	62.14(15)	H(43)a ,	H(63)b	35.97(12)
H(1) ,	H(12)	53.23(9)	H(1) ,	H(611)	104.53(10)	H(1) ,	H(601)	73.42(9)	H(1) ,	H(11)	91.62(9)
H(1) ,	H(31)	125.06(9)	H(1) ,	H(41)	111.18(9)	H(1) ,	H(62)	125.77(9)	H(1) ,	H(4)b	42.92(7)
H(1) ,	H(63)b	56.83(9)	H(12) ,	H(611)	141.66(11)	H(12) ,	H(601)	126.04(10)	H(12) ,	H(11)	39.54(9)
H(12) ,	H(31)	86.62(8)	H(12) ,	H(41)	130.95(10)	H(12) ,	H(62)	172.38(10)	H(12) ,	H(4)b	85.39(7)
H(12) ,	H(63)b	47.43(9)	H(611) ,	H(601)	53.24(11)	H(611) ,	H(11)	150.52(11)	H(611) ,	H(31)	127.87(10)
H(611) ,	H(41)	84.01(10)	H(611) ,	H(62)	31.35(10)	H(611) ,	H(4)b	62.85(9)	H(611) ,	H(63)b	94.82(10)

H(601)	H(11)	156.16(11)	H(601)	H(31)	123.20(9)	H(601)	H(41)	58.35(8)	H(601)	H(62)	55.05(9)
H(601)	H(4)b	56.06(8)	H(601)	H(63)b	111.07(9)	H(11)	H(31)	51.28(8)	H(11)	H(41)	113.27(9)
H(11)	H(62)	142.60(10)	H(11)	H(4)b	123.46(8)	H(11)	H(63)b	73.37(9)	H(31)	H(41)	65.22(7)
H(31)	H(62)	98.75(8)	H(31)	H(4)b	167.76(8)	H(31)	H(63)b	123.84(8)	H(41)	H(62)	56.61(8)
H(41)	H(4)b	114.04(7)	H(41)	H(63)b	167.32(9)	H(62)	H(4)b	90.14(7)	H(62)	H(63)b	125.04(9)
H(4)b	H(63)b	55.01(7)									

3.6 Angstrom Coordination Sphere Around Atom I = O(31) [ARU = 1555.01] -0.07367 0.31776 0.20452 -1.1558 2.7661 1.5464

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.969(3)	--	H(301)	[=	]	Intra	57.12	-12.81	-0.03100	0.40890	0.17610	-0.6428	3.5595	1.3315
2	1.4031(18)	--	C(31)	[=	]	Intra	-52.11	3.19	0.00718	0.19075	0.21485	-0.2954	1.6605	1.6245
3	2.4755(17)	<<	C(41)	[=	]	Intra	-36.73	-27.22	0.06478	0.16653	0.05476	0.6086	1.4496	0.4141
4	2.4933(16)	<<	C(21)	[=	]	Intra	-30.27	29.91	0.12446	0.19262	0.36895	0.7108	1.6768	2.7897
5	2.7435(16)	<<	O(1)	[=	]	Intra	6.07	31.05	0.17143	0.34630	0.39165	1.1816	3.0145	2.9614
6	2.8618(19)	.<	O(3)a	[-x,-1/2+y,1-z =	2546.01]		-167.30	14.17	-0.30801	0.24770	0.29720	-3.8625	2.1562	2.2472
7	2.864(2)	.<	O(41)b	[-x,1/2+y,-z =	2555.01]		63.16	-17.75	0.02123	0.59734	0.08904	0.0759	5.1998	0.6733
8	3.1265(19)	..	O(41)	[=	]	Intra	-60.63	-45.23	-0.02123	0.09734	-0.08904	-0.0759	0.8473	-0.6733
9	3.2561(18)	..	O(11)	[=	]	Intra	-60.58	75.38	0.03017	0.23550	0.62119	-0.7519	2.0500	4.6970
10	3.3150(17)	..	C(11)	[=	]	Intra	-50.71	50.70	0.10301	0.13110	0.54380	0.1739	1.1412	4.1118
11	3.3361(17)	..	C(51)b	[-x,1/2+y,-z =	2555.01]		104.20	-49.04	-0.17635	0.56133	-0.12864	-1.6922	4.8864	-0.9727
12	3.4108(18)	..	C(11)c	[-x,1/2+y,1-z =	2556.01]		105.49	33.91	-0.10301	0.63110	0.45620	-1.9119	5.4937	3.4495
13	3.5394(18)	..	C(61)b	[-x,1/2+y,-z =	2555.01]		129.65	-32.46	-0.28927	0.58194	-0.04668	-3.0613	5.0658	-0.3530
14	3.5827(17)	..	C(3)a	[-x,-1/2+y,1-z =	2546.01]		-149.75	29.18	-0.28545	0.13673	0.43553	-3.8579	1.1902	3.2932
15	3.5996(18)	..	O(21)	[=	]	Intra	-33.74	13.51	0.21205	0.09445	0.31572	1.7548	0.8222	2.3873
16	1.907(4)	<<	H(33)a	[-x,-1/2+y,1-z =	2546.01]		-166.02	12.10	-0.23180	0.26600	0.25740	-2.9655	2.3155	1.9463
17	2.017(3)	<<	H(31)	[=	]	Intra	-83.71	5.27	-0.04950	0.08840	0.22900	-0.9357	0.7695	1.7315
18	2.639(3)	.<	H(51)b	[-x,1/2+y,-z =	2555.01]		102.64	-65.57	-0.14650	0.44010	-0.11330	-1.3946	3.8311	-0.8567
19	2.645(3)	.<	H(41)	[=	]	Intra	-9.13	-32.70	0.09840	0.27720	0.01550	1.0420	2.4130	0.1172
20	2.742(3)	..	H(11)c	[-x,1/2+y,1-z =	2556.01]		97.69	49.04	-0.05200	0.52240	0.47840	-1.3964	4.5475	3.6173
21	2.834(4)	..	H(62)b	[-x,1/2+y,-z =	2555.01]		134.17	-18.00	-0.26510	0.53990	0.08870	-3.0340	4.6998	0.6707
22	3.091(3)	..	H(401)b	[-x,1/2+y,-z =	2555.01]		71.19	-1.18	0.01670	0.65380	0.19610	-0.1594	5.6913	1.4828
23	3.239(3)	..	H(12)c	[-x,1/2+y,1-z =	2556.01]		122.20	22.29	-0.19470	0.60910	0.36700	-2.7529	5.3022	2.7750
24	3.275(3)	..	H(3)a	[-x,-1/2+y,1-z =	2546.01]		-139.51	44.92	-0.18710	0.14480	0.51030	-2.9194	1.2605	3.8585
25	3.527(3)	..	H(101)	[=	]	Intra	3.69	74.57	0.08450	0.32470	0.65420	-0.2191	2.8265	4.9466
26	3.598(3)	..	H(401)	[=	]	Intra	-47.34	-57.35	-0.01670	0.15380	-0.19610	0.1594	1.3388	-1.4828

Angles (Degrees) At1...V...At2 with Vertex V = O(31)

H(301) ,	C(31)	109.45(18)	H(301) ,	C(41)	87.52(16)	H(301) ,	C(21)	94.13(16)	H(301) ,	O(1)	65.75(15)
H(301) ,	O(3)a	136.85(18)	H(301) ,	O(41)b	7.64(15)	H(301) ,	O(41)	99.34(16)	H(301) ,	O(11)	109.21(16)
H(301) ,	C(11)	111.14(16)	H(301) ,	C(51)b	52.93(15)	H(301) ,	C(11)c	65.56(16)	H(301) ,	C(61)b	68.53(16)
H(301) ,	C(3)a	150.18(17)	H(301) ,	O(21)	93.78(16)	H(301) ,	H(33)a	137.9(2)	H(301) ,	H(31)	140.63(19)
H(301) ,	H(51)b	61.02(16)	H(301) ,	H(41)	63.23(16)	H(301) ,	H(11)c	71.46(17)	H(301) ,	H(62)b	73.96(17)
H(301) ,	H(401)b	18.16(16)	H(301) ,	H(12)c	72.78(17)	H(301) ,	H(3)a	144.91(17)	H(301) ,	H(101)	93.39(16)
H(301) ,	H(401)	86.82(16)	C(31) ,	C(41)	33.84(5)	C(31) ,	C(21)	33.79(5)	C(31) ,	O(1)	61.33(7)
C(31) ,	O(3)a	113.48(9)	C(31) ,	O(41)b	115.02(8)	C(31) ,	O(41)	49.01(6)	C(31) ,	O(11)	72.35(7)
C(31) ,	C(11)	47.53(6)	C(31) ,	C(51)b	129.90(8)	C(31) ,	C(11)c	137.31(8)	C(31) ,	C(61)b	150.69(8)
C(31) ,	C(3)a	95.09(8)	C(31) ,	O(21)	20.88(6)	C(31) ,	H(33)a	112.58(14)	C(31) ,	H(31)	31.58(8)
C(31) ,	H(51)b	115.09(10)	C(31) ,	H(41)	54.23(8)	C(31) ,	H(11)c	121.58(10)	C(31) ,	H(62)b	163.97(11)
C(31) ,	H(401)b	123.31(10)	C(31) ,	H(12)c	153.92(9)	C(31) ,	H(3)a	85.91(8)	C(31) ,	H(101)	78.29(8)
C(31) ,	H(401)	60.67(7)	C(41) ,	C(21)	57.47(4)	C(41) ,	O(1)	71.15(5)	C(41) ,	O(3)a	132.28(7)
C(41) ,	O(41)b	90.34(6)	C(41) ,	O(41)	26.19(4)	C(41) ,	O(11)	103.73(5)	C(41) ,	C(11)	78.90(5)

C(41)	, C(51)b	96.15(5)	C(41)	, C(11)c	146.98(6)	C(41)	, C(61)b	118.93(5)	C(41)	, C(3)a	121.78(6)
C(41)	, O(21)	40.83(3)	C(41)	, H(33)a	130.28(13)	C(41)	, H(31)	55.80(8)	C(41)	, H(51)b	82.10(8)
C(41)	, H(41)	24.46(6)	C(41)	, H(11)c	138.89(9)	C(41)	, H(62)b	133.93(8)	C(41)	, H(401)b	105.31(8)
C(41)	, H(12)c	160.27(8)	C(41)	, H(3)a	117.54(7)	C(41)	, H(101)	105.12(7)	C(41)	, H(401)	31.05(5)
C(21)	, O(1)	31.20(4)	C(21)	, O(3)a	119.53(6)	C(21)	, O(41)b	101.62(6)	C(21)	, O(41)	80.06(5)
C(21)	, O(11)	47.82(4)	C(21)	, C(11)	25.80(3)	C(21)	, C(51)b	140.77(6)	C(21)	, C(11)c	103.72(5)

C(21)	C(61)b	162.65(6)	C(21)	C(3)a	97.43(5)	C(21)	O(21)	16.71(3)	C(21)	H(33)a	120.17(12)
C(21)	H(31)	55.95(8)	C(21)	H(51)b	134.27(9)	C(21)	H(41)	65.74(6)	C(21)	H(11)c	88.45(8)
C(21)	H(62)b	161.48(9)	C(21)	H(401)b	100.51(7)	C(21)	H(12)c	121.47(6)	C(21)	H(3)a	81.39(6)
C(21)	H(101)	47.78(6)	C(21)	H(401)	88.45(6)	O(1)	O(3)a	134.33(6)	O(1)	O(41)b	73.38(5)
O(1)	O(41)	97.32(5)	O(1)	O(11)	54.21(4)	O(1)	C(11)	45.86(4)	O(1)	C(51)b	117.96(5)
O(1)	C(11)c	80.14(5)	O(1)	C(61)b	132.58(6)	O(1)	C(3)a	115.53(5)	O(1)	O(21)	40.50(4)
O(1)	H(33)a	136.19(11)	O(1)	H(31)	87.10(8)	O(1)	H(51)b	120.67(9)	O(1)	H(41)	65.35(6)
O(1)	H(11)c	68.07(8)	O(1)	H(62)b	131.46(9)	O(1)	H(401)b	69.53(7)	O(1)	H(12)c	98.83(6)
O(1)	H(3)a	97.84(6)	O(1)	H(101)	43.54(6)	O(1)	H(401)	99.13(7)	O(3)a	O(41)b	131.49(7)
O(3)a	O(41)	111.70(6)	O(3)a	O(11)	80.42(5)	O(3)a	C(11)	94.90(5)	O(3)a	C(51)b	99.69(5)
O(3)a	C(11)c	79.87(5)	O(3)a	C(61)b	76.15(5)	O(3)a	C(3)a	22.11(4)	O(3)a	O(21)	126.33(6)
O(3)a	H(33)a	2.42(10)	O(3)a	H(31)	82.52(8)	O(3)a	H(51)b	102.91(9)	O(3)a	H(41)	152.83(8)
O(3)a	H(11)c	82.56(8)	O(3)a	H(62)b	66.06(8)	O(3)a	H(401)b	120.77(8)	O(3)a	H(12)c	66.90(6)
O(3)a	H(3)a	38.71(5)	O(3)a	H(101)	91.08(7)	O(3)a	H(401)	117.87(7)	O(41)b	O(41)	99.01(5)
O(41)b	O(11)	115.38(6)	O(41)b	C(11)	118.68(5)	O(41)b	C(51)b	45.48(4)	O(41)b	C(11)c	65.54(4)
O(41)b	C(61)b	61.04(4)	O(41)b	C(3)a	147.86(6)	O(41)b	O(21)	100.51(5)	O(41)b	H(33)a	132.27(12)
O(41)b	H(31)	145.30(9)	O(41)b	H(51)b	54.44(7)	O(41)b	H(41)	65.88(7)	O(41)b	H(11)c	73.50(7)
O(41)b	H(62)b	67.11(8)	O(41)b	H(401)b	18.35(5)	O(41)b	H(12)c	70.27(7)	O(41)b	H(3)a	146.89(7)
O(41)b	H(101)	99.51(6)	O(41)b	H(401)	85.60(6)	O(41)	O(11)	120.61(6)	O(41)	C(11)	96.32(5)
O(41)	C(51)b	84.81(4)	O(41)	C(11)c	164.47(6)	O(41)	C(61)b	101.75(5)	O(41)	C(3)a	109.68(5)
O(41)	O(21)	63.58(4)	O(41)	H(33)a	109.36(12)	O(41)	H(31)	54.55(8)	O(41)	H(51)b	68.44(7)
O(41)	H(41)	41.19(6)	O(41)	H(11)c	164.83(9)	O(41)	H(62)b	115.35(8)	O(41)	H(401)b	117.06(7)
O(41)	H(12)c	156.94(7)	O(41)	H(3)a	113.90(7)	O(41)	H(101)	127.10(7)	O(41)	H(401)	14.64(5)
O(11)	C(11)	25.00(3)	O(11)	C(51)b	152.92(6)	O(11)	C(11)c	70.34(4)	O(11)	C(61)b	136.80(5)
O(11)	C(3)a	61.65(4)	O(11)	O(21)	63.57(4)	O(11)	H(33)a	82.12(10)	O(11)	H(31)	71.34(8)
O(11)	H(51)b	168.80(9)	O(11)	H(41)	112.98(7)	O(11)	H(11)c	54.76(7)	O(11)	H(62)b	122.09(8)
O(11)	H(401)b	100.84(6)	O(11)	H(12)c	82.32(6)	O(11)	H(3)a	44.15(5)	O(11)	H(101)	15.87(5)
O(11)	H(401)	133.01(7)	C(11)	C(51)b	163.82(5)	C(11)	C(11)c	92.82(4)	C(11)	C(61)b	161.75(5)
C(11)	C(3)a	73.12(4)	C(11)	O(21)	39.67(3)	C(11)	H(33)a	95.89(11)	C(11)	H(31)	53.14(7)
C(11)	H(51)b	159.83(9)	C(11)	H(41)	91.11(7)	C(11)	H(11)c	76.66(7)	C(11)	H(62)b	147.06(8)
C(11)	H(401)b	110.52(7)	C(11)	H(12)c	106.74(6)	C(11)	H(3)a	56.24(5)	C(11)	H(101)	32.43(5)
C(11)	H(401)	108.09(6)	C(51)b	C(11)c	82.96(4)	C(51)b	C(61)b	25.21(3)	C(51)b	C(3)a	121.77(4)
C(51)b	O(21)	130.51(4)	C(51)b	H(33)a	98.97(11)	C(51)b	H(31)	135.72(9)	C(51)b	H(51)b	16.56(6)
C(51)b	H(41)	79.07(6)	C(51)b	H(11)c	98.24(8)	C(51)b	H(62)b	39.34(7)	C(51)b	H(401)b	55.58(6)
C(51)b	H(12)c	73.11(6)	C(51)b	H(3)a	137.63(6)	C(51)b	H(101)	139.44(7)	C(51)b	H(401)	71.04(5)
C(11)c	C(61)b	70.15(4)	C(11)c	C(3)a	84.98(4)	C(11)c	O(21)	118.74(4)	C(11)c	H(33)a	82.04(11)
C(11)c	H(31)	139.87(8)	C(11)c	H(51)b	99.51(7)	C(11)c	H(41)	126.33(8)	C(11)c	H(11)c	16.20(7)
C(11)c	H(62)b	58.66(7)	C(11)c	H(401)b	47.63(6)	C(11)c	H(12)c	18.72(5)	C(11)c	H(3)a	81.62(6)
C(11)c	H(101)	60.48(5)	C(11)c	H(401)	150.24(6)	C(61)b	C(3)a	98.13(4)	C(61)b	O(21)	155.72(5)
C(61)b	H(33)a	75.83(11)	C(61)b	H(31)	138.68(9)	C(61)b	H(51)b	36.92(7)	C(61)b	H(41)	104.13(7)
C(61)b	H(11)c	86.33(8)	C(61)b	H(62)b	15.02(7)	C(61)b	H(401)b	63.10(6)	C(61)b	H(12)c	55.21(5)
C(61)b	H(3)a	112.81(6)	C(61)b	H(101)	130.48(6)	C(61)b	H(401)	90.16(6)	C(3)a	O(21)	104.98(4)
C(3)a	H(33)a	22.82(10)	C(3)a	H(31)	66.56(8)	C(3)a	H(51)b	123.58(8)	C(3)a	H(41)	146.23(8)
C(3)a	H(11)c	81.45(7)	C(3)a	H(62)b	87.19(8)	C(3)a	H(401)b	132.02(7)	C(3)a	H(12)c	77.74(6)
C(3)a	H(3)a	17.70(4)	C(3)a	H(101)	74.80(6)	C(3)a	H(401)	120.78(6)	O(21)	H(33)a	126.20(12)
O(21)	H(31)	49.90(7)	O(21)	H(51)b	120.25(8)	O(21)	H(41)	51.85(6)	O(21)	H(11)c	104.20(8)
O(21)	H(62)b	167.53(9)	O(21)	H(401)b	104.79(7)	O(21)	H(12)c	137.13(6)	O(21)	H(3)a	91.28(6)
O(21)	H(101)	64.49(6)	O(21)	H(401)	71.75(6)	H(33)a	H(31)	81.40(13)	H(33)a	H(51)b	101.56(13)
H(33)a	H(41)	150.46(13)	H(33)a	H(11)c	84.95(13)	H(33)a	H(62)b	66.25(13)	H(33)a	H(401)b	122.26(13)

H(33)a ,	H(12)c	68.75(12)	H(33)a ,	H(3)a	39.86(11)	H(33)a ,	H(101)	93.09(11)	H(33)a ,	H(401)	115.45(12)
H(31) ,	H(51)b	119.52(10)	H(31) ,	H(41)	80.03(10)	H(31) ,	H(11)c	125.68(10)	H(31) ,	H(62)b	140.89(11)
H(31) ,	H(401)b	154.62(10)	H(31) ,	H(12)c	142.55(10)	H(31) ,	H(3)a	62.54(8)	H(31) ,	H(101)	84.23(9)
H(31) ,	H(401)	69.19(8)	H(51)b ,	H(41)	68.72(9)	H(51)b ,	H(11)c	114.68(10)	H(51)b ,	H(62)b	51.94(9)
H(51)b ,	H(401)b	68.19(8)	H(51)b ,	H(12)c	89.13(8)	H(51)b ,	H(3)a	141.23(9)	H(51)b ,	H(101)	153.48(9)
H(51)b ,	H(401)	55.01(8)	H(41) ,	H(11)c	124.58(10)	H(41) ,	H(62)b	118.34(10)	H(41) ,	H(401)b	81.22(9)
H(41) ,	H(12)c	135.98(9)	H(41) ,	H(3)a	140.14(9)	H(41) ,	H(101)	107.61(8)	H(41) ,	H(401)	35.75(7)

H(11)c ,	H(62)b	74.46(10)	H(11)c ,	H(401)b	55.18(8)	H(11)c ,	H(12)c	33.04(8)	H(11)c ,	H(3)a	73.63(8)
H(11)c ,	H(101)	44.29(8)	H(11)c ,	H(401)	157.77(9)	H(62)b ,	H(401)b	64.00(10)	H(62)b ,	H(12)c	41.95(8)
H(62)b ,	H(3)a	100.07(9)	H(62)b ,	H(101)	117.52(9)	H(62)b ,	H(401)	104.64(8)	H(401)b,	H(12)c	54.95(8)
H(401)b,	H(3)a	128.56(8)	H(401)b,	H(101)	85.30(7)	H(401)b,	H(401)	103.90(7)	H(12)c ,	H(3)a	80.02(7)
H(12)c ,	H(101)	75.64(7)	H(12)c ,	H(401)	144.12(7)	H(3)a ,	H(101)	58.01(7)	H(3)a ,	H(401)	127.52(8)
H(101) ,	H(401)	136.17(8)									

3.6 Angstrom Coordination Sphere Around Atom I = O(41) [ARU = 1555.01] -0.02123 0.09734 -0.08904 -0.0759 0.8473 -0.6733

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.976(3)	--	H(401)			Intra	64.42	-56.05	-0.01670	0.15380	-0.19610	0.1594	1.3388	-1.4828
2	1.4190(16)	--	C(41)			Intra	41.35	50.02	0.06478	0.16653	0.05476	0.6086	1.4496	0.4141
3	2.4359(16)	<<	C(51)			Intra	-10.05	42.51	0.17635	0.06133	0.12864	1.6922	0.5339	0.9727
4	2.4473(15)	<<	C(31)			Intra	105.11	69.87	0.00718	0.19075	0.21485	-0.2954	1.6605	1.6245
5	2.7157(18)	<<	O(11)a	x,y,-1+z	1554.01		48.55	-53.79	0.03017	0.23550	-0.37881	0.9861	2.0500	-2.8643
6	2.864(2)	.<	O(31)b	-x,-1/2+y,-z	2545.01		-63.16	-17.75	0.07367	-0.18224	-0.20452	1.1558	-1.5864	-1.5464
7	3.1265(19)	..	O(31)			Intra	119.37	45.23	-0.07367	0.31776	0.20452	-1.1558	2.7661	1.5464
8	3.3035(17)	..	C(61)			Intra	-2.45	18.10	0.28927	0.08194	0.04668	3.0613	0.7133	0.3530
9	3.3517(18)	..	O(1)b	-x,-1/2+y,-z	2545.01		-116.84	-43.05	-0.17143	-0.15370	-0.39165	-1.1816	-1.3380	-2.9614
10	3.4271(15)	..	C(11)a	x,y,-1+z	1554.01		8.41	-54.10	0.10301	0.13110	-0.45620	1.9119	1.1412	-3.4495
11	3.5664(15)	..	O(21)			Intra	-0.79	59.11	0.21205	0.09445	0.31572	1.7548	0.8222	2.3873
12	1.908(3)	<<	H(301)b	-x,-1/2+y,-z	2545.01		-66.34	-20.18	0.03100	-0.09110	-0.17610	0.6428	-0.7930	-1.3315
13	2.080(3)	<<	H(41)			Intra	54.47	22.34	0.09840	0.27720	0.01550	1.0420	2.4130	0.1172
14	2.525(3)	.<	H(51)			Intra	-42.95	37.29	0.14650	-0.05990	0.11330	1.3946	-0.5214	0.8567
15	2.555(3)	.<	H(31)			Intra	-174.83	70.25	-0.04950	0.08840	0.22900	-0.9357	0.7695	1.7315
16	2.610(3)	.<	H(5)b	-x,-1/2+y,-z	2545.01		-172.63	-20.39	-0.26380	0.06130	-0.20930	-2.5020	0.5336	-1.5826
17	3.001(3)	..	H(41)b	-x,-1/2+y,-z	2545.01		-109.12	10.68	-0.09840	-0.22280	-0.01550	-1.0420	-1.9395	-0.1172
18	3.150(4)	..	H(62)			Intra	-9.13	0.05	0.26510	0.03990	-0.08870	3.0340	0.3473	-0.6707
19	3.198(3)	..	H(101)a	x,y,-1+z	1554.01		51.14	-37.37	0.08450	0.32470	-0.34580	1.5190	2.8265	-2.6147
20	3.251(3)	..	H(3)b	-x,-1/2+y,-z	2545.01		159.51	-68.72	-0.18710	0.14480	-0.48970	-1.1814	1.2605	-3.7028
21	3.267(3)	..	H(51)c	-x,1/2+y,-z	2555.01		113.84	-3.22	-0.14650	0.44010	-0.11330	-1.3946	3.8311	-0.8567
22	3.356(3)	..	H(11)a	x,y,-1+z	1554.01		-23.90	-61.32	0.05200	0.02240	-0.47840	1.3964	0.1950	-3.6173
23	3.420(3)	..	H(301)			Intra	101.81	35.89	-0.03100	0.40890	0.17610	-0.6428	3.5595	1.3315
24	3.526(3)	..	H(12)a	x,y,-1+z	1554.01		2.07	-36.59	0.19470	0.10910	-0.36700	2.7529	0.9497	-2.7750

Angles (Degrees) At1...V...At2 with Vertex V = O(41)

H(401)	C(41)	107.8(2)	H(401)	C(51)	116.8(2)	H(401)	C(31)	129.29(19)	H(401)	O(11)a	9.4(2)
H(401)	O(31)b	94.09(18)	H(401)	O(31)	111.29(19)	H(401)	C(61)	92.8(2)	H(401)	O(1)b	80.89(17)
H(401)	C(11)a	31.23(19)	H(401)	O(21)	126.3(2)	H(401)	H(301)b	93.21(19)	H(401)	H(41)	78.85(19)
H(401)	H(51)	129.4(2)	H(401)	H(31)	151.3(2)	H(401)	H(5)b	89.8(2)	H(401)	H(41)b	134.34(19)
H(401)	H(62)	80.9(2)	H(401)	H(101)a	20.70(19)	H(401)	H(3)b	40.97(19)	H(401)	H(51)c	65.84(19)
H(401)	H(11)a	42.63(18)	H(401)	H(301)	97.29(19)	H(401)	H(12)a	45.4(2)	C(41)	C(51)	35.58(7)
C(41)	C(31)	35.19(5)	C(41)	O(11)a	103.98(9)	C(41)	O(31)b	112.76(9)	C(41)	O(31)	50.36(7)
C(41)	C(61)	47.24(6)	C(41)	O(1)b	163.54(10)	C(41)	C(11)a	107.73(8)	C(41)	O(21)	25.55(7)
C(41)	H(301)b	116.59(12)	C(41)	H(41)	29.54(9)	C(41)	H(51)	59.00(9)	C(41)	H(31)	56.91(8)
C(41)	H(5)b	140.03(10)	C(41)	H(41)b	114.04(9)	C(41)	H(62)	65.83(9)	C(41)	H(101)a	87.82(9)
C(41)	H(3)b	145.50(11)	C(41)	H(51)c	81.38(10)	C(41)	H(11)a	122.90(10)	C(41)	H(301)	45.10(8)
C(41)	H(12)a	93.29(8)	C(51)	C(31)	58.23(4)	C(51)	O(11)a	108.56(6)	C(51)	O(31)b	77.56(6)
C(51)	O(31)	81.37(5)	C(51)	C(61)	25.25(3)	C(51)	O(1)b	128.09(7)	C(51)	C(11)a	97.90(5)
C(51)	O(21)	17.56(3)	C(51)	H(301)b	81.32(9)	C(51)	H(41)	56.63(8)	C(51)	H(51)	25.60(7)
C(51)	H(31)	66.70(6)	C(51)	H(5)b	153.47(8)	C(51)	H(41)b	89.37(7)	C(51)	H(62)	42.47(6)
C(51)	H(101)a	97.35(7)	C(51)	H(3)b	153.23(7)	C(51)	H(51)c	116.64(8)	C(51)	H(11)a	104.44(7)

C(51)	H(301)	80.00(6)	C(51)	H(12)a	79.87(6)	C(31)	O(11)a	130.20(8)	C(31)	O(31)b	127.39(6)
C(31)	O(31)	25.64(4)	C(31)	C(61)	78.87(4)	C(31)	O(1)b	145.90(6)	C(31)	C(11)a	141.64(6)
C(31)	O(21)	40.77(3)	C(31)	H(301)b	130.04(10)	C(31)	H(41)	56.03(7)	C(31)	H(51)	70.33(7)
C(31)	H(31)	25.34(6)	C(31)	H(5)b	106.48(7)	C(31)	H(41)b	96.07(7)	C(31)	H(62)	98.08(7)
C(31)	H(101)a	114.15(8)	C(31)	H(3)b	143.34(8)	C(31)	H(51)c	73.33(6)	C(31)	H(11)a	158.08(8)
C(31)	H(301)	34.03(5)	C(31)	H(12)a	128.47(7)	O(11)a	O(31)b	87.83(6)	O(11)a	O(31)	115.85(7)

O(11)a ,	C(61)	84.10(5)	O(11)a ,	O(1)b	82.36(5)	O(11)a ,	C(11)a	23.31(4)	O(11)a ,	O(21)	119.65(6)
O(11)a ,	H(301)b	87.43(9)	O(11)a ,	H(41)	76.29(8)	O(11)a ,	H(51)	120.08(9)	O(11)a ,	H(31)	154.75(10)
O(11)a ,	H(5)b	97.80(7)	O(11)a ,	H(41)b	133.36(7)	O(11)a ,	H(62)	71.63(7)	O(11)a ,	H(101)a	16.51(6)
O(11)a ,	H(3)b	47.54(5)	O(11)a ,	H(51)c	73.03(7)	O(11)a ,	H(11)a	37.50(6)	O(11)a ,	H(301)	100.75(7)
O(11)a ,	H(12)a	36.14(6)	O(31)b ,	O(31)	152.44(6)	O(31)b ,	C(61)	69.62(5)	O(31)b ,	O(1)b	51.66(4)
O(31)b ,	C(11)a	64.94(4)	O(31)b ,	O(21)	92.00(5)	O(31)b ,	H(301)b	3.87(7)	O(31)b ,	H(41)	121.63(9)
O(31)b ,	H(51)	58.24(7)	O(31)b ,	H(31)	113.94(8)	O(31)b ,	H(5)b	101.03(8)	O(31)b ,	H(41)b	53.55(6)
O(31)b ,	H(62)	56.00(7)	O(31)b ,	H(101)a	97.26(7)	O(31)b ,	H(3)b	88.29(6)	O(31)b ,	H(51)c	158.82(6)
O(31)b ,	H(11)a	51.58(6)	O(31)b ,	H(301)	157.50(6)	O(31)b ,	H(12)a	59.86(7)	O(31) ,	C(61)	97.61(5)
O(31) ,	O(1)b	140.43(5)	O(31) ,	C(11)a	136.29(6)	O(31) ,	O(21)	64.68(4)	O(31) ,	H(301)b	154.51(9)
O(31) ,	H(41)	56.90(7)	O(31) ,	H(51)	95.95(7)	O(31) ,	H(31)	40.03(7)	O(31) ,	H(5)b	90.00(7)
O(31) ,	H(41)b	109.09(6)	O(31) ,	H(62)	115.97(7)	O(31) ,	H(101)a	102.91(7)	O(31) ,	H(3)b	117.78(7)
O(31) ,	H(51)c	48.70(5)	O(31) ,	H(11)a	153.35(8)	O(31) ,	H(301)	16.23(5)	O(31) ,	H(12)a	133.04(8)
C(61) ,	O(1)b	119.93(5)	C(61) ,	C(11)a	72.80(4)	C(61) ,	O(21)	41.03(3)	C(61) ,	H(301)b	73.42(8)
C(61) ,	H(41)	53.28(8)	C(61) ,	H(51)	40.25(8)	C(61) ,	H(31)	91.49(6)	C(61) ,	H(5)b	170.46(9)
C(61) ,	H(41)b	102.15(7)	C(61) ,	H(62)	19.21(6)	C(61) ,	H(101)a	74.94(7)	C(61) ,	H(3)b	128.14(6)
C(61) ,	H(51)c	115.96(8)	C(61) ,	H(11)a	81.26(7)	C(61) ,	H(301)	90.43(5)	C(61) ,	H(12)a	54.86(5)
O(1)b ,	C(11)a	72.20(4)	O(1)b ,	O(21)	138.64(6)	O(1)b ,	H(301)b	47.79(8)	O(1)b ,	H(41)	158.06(8)
O(1)b ,	H(51)	104.61(8)	O(1)b ,	H(31)	120.77(8)	O(1)b ,	H(5)b	51.47(6)	O(1)b ,	H(41)b	54.19(5)
O(1)b ,	H(62)	102.87(7)	O(1)b ,	H(101)a	98.83(6)	O(1)b ,	H(3)b	48.28(5)	O(1)b ,	H(51)c	115.08(6)
O(1)b ,	H(11)a	54.48(6)	O(1)b ,	H(301)	149.60(6)	O(1)b ,	H(12)a	82.92(6)	C(11)a ,	O(21)	113.46(4)
C(11)a ,	H(301)b	64.90(8)	C(11)a ,	H(41)	86.08(8)	C(11)a ,	H(51)	101.51(8)	C(11)a ,	H(31)	163.79(7)
C(11)a ,	H(5)b	105.50(6)	C(11)a ,	H(41)b	114.61(7)	C(11)a ,	H(62)	56.06(6)	C(11)a ,	H(101)a	33.49(5)
C(11)a ,	H(3)b	55.35(5)	C(11)a ,	H(51)c	96.33(6)	C(11)a ,	H(11)a	18.47(5)	C(11)a ,	H(301)	120.20(6)
C(11)a ,	H(12)a	18.05(4)	O(21) ,	H(301)b	95.55(9)	O(21) ,	H(41)	53.36(7)	O(21) ,	H(51)	34.65(6)
O(21) ,	H(31)	50.57(6)	O(21) ,	H(5)b	140.84(7)	O(21) ,	H(41)b	89.98(6)	O(21) ,	H(62)	59.43(6)
O(21) ,	H(101)a	105.62(7)	O(21) ,	H(3)b	167.18(7)	O(21) ,	H(51)c	105.18(6)	O(21) ,	H(11)a	121.76(7)
O(21) ,	H(301)	65.65(5)	O(21) ,	H(12)a	95.73(5)	H(301)b,	H(41)	125.16(12)	H(301)b,	H(51)	61.56(10)
H(301)b,	H(31)	115.17(11)	H(301)b,	H(5)b	97.27(10)	H(301)b,	H(41)b	52.19(9)	H(301)b,	H(62)	59.46(10)
H(301)b,	H(101)a	97.74(10)	H(301)b,	H(3)b	85.17(9)	H(301)b,	H(51)c	156.60(9)	H(301)b,	H(11)a	50.57(9)
H(301)b,	H(301)	161.16(10)	H(301)b,	H(12)a	61.12(10)	H(41) ,	H(51)	82.23(10)	H(41) ,	H(31)	81.15(9)
H(41) ,	H(5)b	136.27(11)	H(41) ,	H(41)b	143.28(9)	H(41) ,	H(62)	65.70(10)	H(41) ,	H(101)a	59.79(9)
H(41) ,	H(3)b	116.18(10)	H(41) ,	H(51)c	63.31(9)	H(41) ,	H(11)a	104.12(9)	H(41) ,	H(301)	43.06(8)
H(41) ,	H(12)a	76.91(9)	H(51) ,	H(31)	67.00(9)	H(51) ,	H(5)b	133.41(11)	H(51) ,	H(41)b	64.65(9)
H(51) ,	H(62)	48.59(9)	H(51) ,	H(101)a	114.38(10)	H(51) ,	H(3)b	146.25(9)	H(51) ,	H(51)c	139.82(9)
H(51) ,	H(11)a	99.83(9)	H(51) ,	H(301)	99.86(8)	H(51) ,	H(12)a	84.82(9)	H(31) ,	H(5)b	90.65(8)
H(31) ,	H(41)b	71.88(8)	H(31) ,	H(62)	109.07(8)	H(31) ,	H(101)a	139.28(9)	H(31) ,	H(3)b	140.03(8)
H(31) ,	H(51)c	86.84(8)	H(31) ,	H(11)a	165.34(10)	H(31) ,	H(301)	54.31(8)	H(31) ,	H(12)a	146.30(8)
H(5)b ,	H(41)b	69.74(8)	H(5)b ,	H(62)	154.03(9)	H(5)b ,	H(101)a	109.05(9)	H(5)b ,	H(3)b	51.28(7)
H(5)b ,	H(51)c	73.44(9)	H(5)b ,	H(11)a	94.52(8)	H(5)b ,	H(301)	98.36(8)	H(5)b ,	H(12)a	122.80(7)
H(41)b ,	H(62)	99.80(9)	H(41)b ,	H(101)a	147.94(8)	H(41)b ,	H(3)b	100.44(7)	H(41)b ,	H(51)c	136.75(8)
H(41)b ,	H(11)a	97.08(8)	H(41)b ,	H(301)	125.05(7)	H(41)b ,	H(12)a	113.31(8)	H(62) ,	H(101)a	66.82(9)
H(62) ,	H(3)b	110.89(8)	H(62) ,	H(51)c	122.92(10)	H(62) ,	H(11)a	62.40(8)	H(62) ,	H(301)	106.80(8)
H(62) ,	H(12)a	38.09(7)	H(101)a,	H(3)b	61.66(7)	H(101)a,	H(51)c	66.55(8)	H(101)a,	H(11)a	50.87(7)
H(101)a,	H(301)	87.01(7)	H(101)a,	H(12)a	38.75(8)	H(3)b ,	H(51)c	72.21(7)	H(3)b ,	H(11)a	49.94(7)
H(3)b ,	H(301)	112.90(7)	H(3)b ,	H(12)a	73.36(6)	H(51)c ,	H(11)a	107.78(7)	H(51)c ,	H(301)	40.69(6)
H(51)c ,	H(12)a	105.30(8)	H(11)a ,	H(301)	137.83(8)	H(11)a ,	H(12)a	29.61(7)	H(301) ,	H(12)a	117.35(8)

3.6 Angstrom Coordination Sphere Around Atom I = O(61) [ARU = 1555.01]   0.32644 0.23800 0.04035   3.4761 2.0718 0.3051

Nr	d(I,J)	To	Atom J	Symm_Oper. on Atom J	ARU(J)	Type	Phi	Mu	X	Y	Z	XO	YO	ZO
1	0.972(3)	--	H(601)	[=	]	Intra	86.31	68.96	0.34770	0.27800	0.16030	3.4986	2.4200	1.2121
2	1.421(2)	--	C(61)	[=	]	Intra	-106.98	1.93	0.28927	0.08194	0.04668	3.0613	0.7133	0.3530
3	2.4481(19)	<<	C(51)	[=	]	Intra	-139.24	15.82	0.17635	0.06133	0.12864	1.6922	0.5339	0.9727
4	2.8497(19)	.<	O(5)	[=	]	Intra	90.79	60.58	0.37719	0.39878	0.36864	3.4568	3.4714	2.7874
5	2.855(2)	.<	O(2)a	[x,y,-1+z =	1554.01]		107.56	-50.83	0.22954	0.43550	-0.25234	2.9321	3.7910	-1.9080
6	2.9363(18)	<<	C(41)	[=	]	Intra	-167.76	2.13	0.06478	0.16653	0.05476	0.6086	1.4496	0.4141
7	2.9765(18)	.<	O(21)	[=	]	Intra	-144.02	44.39	0.21205	0.09445	0.31572	1.7548	0.8222	2.3873
8	3.311(2)	..	C(6)	[=	]	Intra	67.95	19.23	0.45754	0.57083	0.18455	4.6496	4.9691	1.3954
9	3.339(2)	..	C(5)	[=	]	Intra	91.82	35.26	0.35925	0.55107	0.29529	3.3894	4.7971	2.2328
10	3.372(2)	..	O(6)b	[1-x,-1/2+y,-z =	2645.01]		-46.93	-47.08	0.41856	0.04530	-0.28620	5.0444	0.3943	-2.1641
11	3.5361(19)	..	C(6)b	[1-x,-1/2+y,-z =	2645.01]		-27.99	-28.75	0.54246	0.07083	-0.18455	6.2137	0.6166	-1.3954
12	1.892(3)	<<	H(23)a	[x,y,-1+z =	1554.01]		102.33	-50.74	0.27190	0.37240	-0.15340	3.2203	3.2417	-1.1599
13	2.030(4)	<<	H(62)	[=	]	Intra	-104.38	-28.73	0.26510	0.03990	-0.08870	3.0340	0.3473	-0.6707
14	2.080(4)	<<	H(611)	[=	]	Intra	-81.18	16.72	0.36720	0.01190	0.11950	3.7813	0.1036	0.9036
15	2.465(3)	<<	H(41)	[=	]	Intra	172.02	-4.37	0.09840	0.27720	0.01550	1.0420	2.4130	0.1172
16	2.508(4)	<<	H(61)	[=	]	Intra	62.62	5.46	0.43720	0.49270	0.07190	4.6245	4.2890	0.5437
17	3.037(4)	..	H(6)b	[1-x,-1/2+y,-z =	2645.01]		-9.29	-25.80	0.54690	0.18730	-0.13450	6.1749	1.6304	-1.0170
18	3.241(3)	..	H(5)	[=	]	Intra	109.09	23.22	0.26380	0.56130	0.20930	2.5020	4.8861	1.5826
19	3.357(3)	..	H(12)a	[x,y,-1+z =	1554.01]		-122.80	-66.57	0.19470	0.10910	-0.36700	2.7529	0.9497	-2.7750
20	3.371(3)	..	H(51)	[=	]	Intra	-128.75	9.42	0.14650	-0.05990	0.11330	1.3946	-0.5214	0.8567
21	3.531(3)	..	H(2)a	[x,y,-1+z =	1554.01]		53.38	-44.73	0.41160	0.46930	-0.28830	4.9724	4.0853	-2.1799
22	3.593(4)	..	H(61)b	[1-x,-1/2+y,-z =	2645.01]		-37.70	-13.66	0.56280	-0.00730	-0.07190	6.2388	-0.0635	-0.5437
23	3.595(3)	..	H(101)a	[x,y,-1+z =	1554.01]		158.91	-54.31	0.08450	0.32470	-0.34580	1.5190	2.8265	-2.6147

Angles (Degrees) At1...V...At2 with Vertex V = O(61)

H(601) ,	C(61)	108.5(2)	H(601) ,	C(51)	89.3(2)	H(601) ,	O(5)	8.6(2)	H(601) ,	O(2)a	120.8(2)
H(601) ,	C(41)	93.7(2)	H(601) ,	O(21)	60.7(2)	H(601) ,	C(6)	51.0(2)	H(601) ,	C(5)	33.8(2)
H(601) ,	O(6)b	148.3(2)	H(601) ,	C(6)b	125.3(2)	H(601) ,	H(23)a	120.3(3)	H(601) ,	H(62)	139.3(3)
H(601) ,	H(611)	93.8(2)	H(601) ,	H(41)	92.5(2)	H(601) ,	H(61)	65.4(2)	H(601) ,	H(6)b	116.0(2)
H(601) ,	H(5)	47.8(2)	H(601) ,	H(12)a	168.8(2)	H(601) ,	H(51)	97.9(2)	H(601) ,	H(2)a	116.3(2)
H(601) ,	H(61)b	114.6(2)	H(601) ,	H(101)a	134.1(2)	C(61) ,	C(51)	34.68(6)	C(61) ,	O(5)	115.99(9)
C(61) ,	O(2)a	123.10(9)	C(61) ,	C(41)	60.74(7)	C(61) ,	O(21)	53.59(7)	C(61) ,	C(6)	158.26(9)
C(61) ,	C(5)	138.86(9)	C(61) ,	O(6)b	71.63(8)	C(61) ,	C(6)b	81.30(8)	C(61) ,	H(23)a	125.28(14)
C(61) ,	H(62)	30.76(10)	C(61) ,	H(611)	29.37(11)	C(61) ,	H(41)	81.18(10)	C(61) ,	H(61)	167.25(13)
C(61) ,	H(6)b	97.76(11)	C(61) ,	H(5)	136.81(10)	C(61) ,	H(12)a	69.42(9)	C(61) ,	H(51)	22.91(8)
C(61) ,	H(2)a	133.82(9)	C(61) ,	H(61)b	70.39(10)	C(61) ,	H(101)a	93.96(9)	C(51) ,	O(5)	93.79(5)
C(51) ,	O(2)a	116.80(6)	C(51) ,	C(41)	31.26(4)	C(51) ,	O(21)	28.85(4)	C(51) ,	C(6)	135.91(6)
C(51) ,	C(5)	109.66(6)	C(51) ,	O(6)b	103.07(7)	C(51) ,	C(6)b	115.90(7)	C(51) ,	H(23)a	120.07(12)
C(51) ,	H(62)	55.86(10)	C(51) ,	H(611)	55.52(10)	C(51) ,	H(41)	52.28(7)	C(51) ,	H(61)	149.65(10)
C(51) ,	H(6)b	132.44(10)	C(51) ,	H(5)	102.65(7)	C(51) ,	H(12)a	83.30(7)	C(51) ,	H(51)	12.06(6)
C(51) ,	H(2)a	149.20(7)	C(51) ,	H(61)b	104.56(9)	C(51) ,	H(101)a	87.52(7)	O(5) ,	O(2)a	112.22(7)
O(5) ,	C(41)	93.73(5)	O(5) ,	O(21)	65.98(4)	O(5) ,	C(6)	44.41(4)	O(5) ,	C(5)	25.33(4)

O(5)	,	O(6)b	152.29(6)	O(5)	,	C(6)b	128.77(6)	O(5)	,	H(23)a	111.70(12)	O(5)	,	H(62)	146.55(12)
O(5)	,	H(611)	102.42(12)	O(5)	,	H(41)	89.53(7)	O(5)	,	H(61)	59.08(8)	O(5)	,	H(6)b	117.16(8)
O(5)	,	H(5)	39.47(5)	O(5)	,	H(12)a	164.14(8)	O(5)	,	H(51)	103.36(6)	O(5)	,	H(2)a	109.62(7)
O(5)	,	H(61)b	120.18(7)	O(5)	,	H(101)a	126.92(7)	O(2)a	,	C(41)	88.30(5)	O(2)a	,	O(21)	133.23(6)
O(2)a	,	C(6)	78.22(5)	O(2)a	,	C(5)	87.20(6)	O(2)a	,	O(6)b	79.66(5)	O(2)a	,	C(6)b	91.29(5)
O(2)a	,	H(23)a	3.31(11)	O(2)a	,	H(62)	95.59(11)	O(2)a	,	H(611)	145.19(13)	O(2)a	,	H(41)	70.69(7)

O(2)a , H(61)	68.20(9)	O(2)a , H(6)b	85.38(8)	O(2)a , H(5)	74.06(6)	O(2)a , H(12)a	56.56(7)
O(2)a , H(51)	118.20(7)	O(2)a , H(2)a	36.07(5)	O(2)a , H(61)b	108.74(7)	O(2)a , H(101)a	30.71(6)
C(41) , O(21)	47.18(4)	C(41) , C(6)	121.29(6)	C(41) , C(5)	97.25(5)	C(41) , O(6)b	112.08(6)
C(41) , C(6)b	133.37(6)	C(41) , H(23)a	91.59(11)	C(41) , H(62)	67.99(11)	C(41) , H(611)	86.11(11)
C(41) , H(41)	21.23(7)	C(41) , H(61)	129.12(11)	C(41) , H(6)b	148.55(9)	C(41) , H(5)	82.87(6)
C(41) , H(12)a	75.69(5)	C(41) , H(51)	39.45(6)	C(41) , H(2)a	124.11(6)	C(41) , H(61)b	129.32(9)
C(41) , H(101)a	62.81(6)	O(21) , C(6)	110.00(5)	O(21) , C(5)	85.63(5)	O(21) , O(6)b	124.91(7)
O(21) , C(6)b	127.69(6)	O(21) , H(23)a	136.30(12)	O(21) , H(62)	81.59(11)	O(21) , H(611)	59.09(11)
O(21) , H(41)	62.64(7)	O(21) , H(61)	124.70(9)	O(21) , H(6)b	139.23(9)	O(21) , H(5)	85.12(6)
O(21) , H(12)a	112.14(7)	O(21) , H(51)	37.39(5)	O(21) , H(2)a	167.62(7)	O(21) , H(61)b	111.12(8)
O(21) , H(101)a	109.97(7)	C(6) , C(5)	26.47(3)	C(6) , O(6)b	120.77(6)	C(6) , C(6)b	104.13(5)
C(6) , H(23)a	76.22(11)	C(6) , H(62)	168.20(11)	C(6) , H(611)	132.95(12)	C(6) , H(41)	104.71(8)
C(6) , H(61)	14.72(7)	C(6) , H(6)b	87.45(8)	C(6) , H(5)	38.44(5)	C(6) , H(12)a	132.15(8)
C(6) , H(51)	146.96(6)	C(6) , H(2)a	65.33(5)	C(6) , H(61)b	108.98(8)	C(6) , H(101)a	106.07(6)
C(5) , O(6)b	147.22(6)	C(5) , C(6)b	129.31(5)	C(5) , H(23)a	86.49(11)	C(5) , H(62)	164.81(11)
C(5) , H(611)	127.59(12)	C(5) , H(41)	84.57(7)	C(5) , H(61)	40.14(8)	C(5) , H(6)b	113.14(8)
C(5) , H(5)	19.24(4)	C(5) , H(12)a	142.83(8)	C(5) , H(51)	121.16(6)	C(5) , H(2)a	87.24(6)
C(5) , H(61)b	129.89(7)	C(5) , H(101)a	106.46(6)	O(6)b , C(6)b	23.52(3)	O(6)b , H(23)a	78.67(11)
O(6)b , H(62)	47.68(10)	O(6)b , H(611)	70.83(11)	O(6)b , H(41)	118.18(8)	O(6)b , H(61)	107.24(9)
O(6)b , H(6)b	36.46(7)	O(6)b , H(5)	149.37(7)	O(6)b , H(12)a	42.44(5)	O(6)b , H(51)	91.39(7)
O(6)b , H(2)a	64.61(6)	O(6)b , H(61)b	34.29(6)	O(6)b , H(101)a	76.29(6)	C(6)b , H(23)a	89.24(11)
C(6)b , H(62)	65.66(10)	C(6)b , H(611)	68.61(11)	C(6)b , H(41)	141.70(8)	C(6)b , H(61)	93.16(9)
C(6)b , H(6)b	16.87(7)	C(6)b , H(5)	141.23(7)	C(6)b , H(12)a	65.67(5)	C(6)b , H(51)	103.90(7)
C(6)b , H(2)a	64.41(5)	C(6)b , H(61)b	17.57(6)	C(6)b , H(101)a	96.73(6)	H(23)a , H(62)	97.10(14)
H(23)a , H(611)	145.87(16)	H(23)a , H(41)	73.86(12)	H(23)a , H(61)	65.73(13)	H(23)a , H(6)b	82.70(12)
H(23)a , H(5)	74.19(11)	H(23)a , H(12)a	57.80(12)	H(23)a , H(51)	121.26(12)	H(23)a , H(2)a	32.84(11)
H(23)a , H(61)b	106.77(12)	H(23)a , H(101)a	33.68(11)	H(62) , H(611)	50.68(14)	H(62) , H(41)	82.30(12)
H(62) , H(61)	153.67(13)	H(62) , H(6)b	82.00(12)	H(62) , H(5)	149.51(12)	H(62) , H(12)a	39.48(11)
H(62) , H(51)	44.82(10)	H(62) , H(2)a	103.79(11)	H(62) , H(61)b	63.20(12)	H(62) , H(101)a	70.70(11)
H(611) , H(41)	107.33(13)	H(611) , H(61)	137.90(14)	H(611) , H(6)b	81.80(13)	H(611) , H(5)	138.81(12)
H(611) , H(12)a	88.82(13)	H(611) , H(51)	46.80(11)	H(611) , H(2)a	132.84(12)	H(611) , H(61)b	52.61(12)
H(611) , H(101)a	120.82(12)	H(41) , H(61)	109.69(12)	H(41) , H(6)b	149.80(9)	H(41) , H(5)	67.23(8)
H(41) , H(12)a	76.33(8)	H(41) , H(51)	60.61(9)	H(41) , H(2)a	106.61(8)	H(41) , H(61)b	145.43(10)
H(41) , H(101)a	51.06(8)	H(61) , H(6)b	76.29(11)	H(61) , H(5)	48.12(9)	H(61) , H(12)a	118.77(10)
H(61) , H(51)	161.30(10)	H(61) , H(2)a	50.87(8)	H(61) , H(61)b	101.29(11)	H(61) , H(101)a	98.10(10)
H(6)b , H(5)	124.39(9)	H(6)b , H(12)a	75.14(8)	H(6)b , H(51)	120.54(10)	H(6)b , H(2)a	53.13(8)
H(6)b , H(61)b	29.28(9)	H(6)b , H(101)a	99.25(8)	H(5) , H(12)a	125.96(8)	H(5) , H(51)	114.71(8)
H(5) , H(2)a	84.81(7)	H(5) , H(61)b	147.17(9)	H(5) , H(101)a	88.52(7)	H(12)a , H(51)	76.11(7)
H(12)a , H(2)a	68.66(7)	H(12)a , H(61)b	75.54(7)	H(12)a , H(101)a	37.60(7)	H(51) , H(2)a	144.64(7)
H(51) , H(61)b	93.23(9)	H(51) , H(101)a	87.61(7)	H(2)a , H(61)b	81.19(8)	H(2)a , H(101)a	62.58(6)
H(61)b , H(101)a	110.58(8)						

==
Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20, Probe Radius = 1.20 Angstrom.
==

```
:: Grid: Z-Axis Step = 0.0278 = Points  36, Angstrom Step = 0.22
:: Grid: Y-Axis Step = 0.0208 = Points  48, Angstrom Step = 0.18
:: Grid: X-Axis Step = 0.0167 = Points  60, Angstrom Step = 0.18
```

:: Unit cell contains no residual Solvent Accessible Area.

===========
*** N O T I C E ***
===========

- PLATON Reference : Spek, A.L. (1990), Acta Cryst. A46, C-34

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU’s (= Esd’s) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl

- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl

- More INFO can be found on http://www.cryst.chem.uu.nl/platon/

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

```
W: No wavelength given.
-------------------------------------------------------------------------------
N: Number of ignored lines on INPUT ....................................    7
          of which blank in column 1 ...................................    7
```

:: Input Data from File sucrose.spf - Data Type SPF

:: NORMAL END of PLATON run - OUTPUT on FILES sucrose.lis & sucrose.lps

:: SPF File   on :sucrose.eld