Acceleration of a nanomotor

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
     Crystal Structure Center,
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
_publ_contact_author_email           A.Meetsma@fwn.rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'JACS'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  July 7 09:27:43 2004


 Consider this CIF submission for deposition of the
 X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : CP900)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_suppl_publ_number           ?
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;
_publ_section_title_footnote
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;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


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_publ_author_name
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_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
```

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# 4. TEXT

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;
_publ_section_exptl_refinement
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;
 Allen, F.H. (2000). Acta Cryst. B58, 380-388.

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   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
   (Present distributor Kluwer Academic Publishers, Dordrecht).

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   Edited by A.J.C Wilson, Kluwer Academic Publishers,
   Dordrecht, The Netherlands.

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   University of G\"ottingen, Germany, 2001

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 Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

 Spek, A.L. (1990). Acta Cryst. A46, C-34.
```

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 Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
;


_publ_section_figure_captions
;
     Fig. 1. Chemical structural diagram (scheme 1) of the title compound

     Fig. 2. Perspective PLUTO drawing of the molecule illustrating the
             configuration and the adopted numbering scheme.

     Fig. 3. Molecular packing viewed down unit cell axes.

     Fig. 4. Perspective ORTEP drawing of the title compound.
             Displacement ellipsoids for non-H are represented at the 50%
             probability level.
             The H-atoms have been omitted to improve clarity.
;

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# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
'C34 H31 N O4'
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_chemical_formula_structural          ?
_chemical_formula_sum
'C34 H31 N O4'
_chemical_formula_iupac               ?
_chemical_formula_weight                 517.62
_chemical_compound_source            'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
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 C   C    0.0033    0.0016
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# 6. CRYSTAL DATA

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_symmetry_space_group_name_H-M       'P 21/c'
_symmetry_Int_Tables_number                14

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
```

```
 -x,1/2+y,1/2-z
 -x,-y,-z
 x,1/2-y,1/2+z

_cell_length_a                         11.2557(8)
_cell_length_b                         16.854(1)
_cell_length_c                         29.162(2)
_cell_angle_alpha                      90
_cell_angle_beta                       91.056(1)
_cell_angle_gamma                      90
_cell_volume                          5531.2(6)
_cell_formula_units_Z                  8

_cell_measurement_temperature    294(1)
_cell_measurement_reflns_used      8657
_cell_measurement_theta_min        2.30
_cell_measurement_theta_max       21.62
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   8657 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'prism'
_exptl_crystal_colour            'yellow'
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_exptl_crystal_size_min           0.10
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.243
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2192
_exptl_absorpt_coefficient_mu     0.081
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min   0.8812
_exptl_absorpt_correction_T_max   0.9919

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# 7. EXPERIMENTAL DATA

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; ?
;
_diffrn_ambient_temperature            294(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method            'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
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_diffrn_detector_area_resol_mean     '4096x4096 / 62x62 (binned 512)'

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loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              54188
_diffrn_reflns_av_R_equivalents    0.0892
_diffrn_reflns_av_sigmaI/netI      0.0830
_diffrn_reflns_limit_h_min         -13
_diffrn_reflns_limit_h_max         13
_diffrn_reflns_limit_k_min         -20
_diffrn_reflns_limit_k_max         20
_diffrn_reflns_limit_l_min         -35
_diffrn_reflns_limit_l_max         35
_diffrn_reflns_theta_min           2.30
_diffrn_reflns_theta_max           25.51
_diffrn_measured_fraction_theta_max    0.994
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.995

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt                  4779
_reflns_threshold_expression       I>2\s(I)


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_computing_cell_refinement          'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction           'XPREP, Bruker Version 5.1/NT, 2000'

_computing_structure_solution
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 SHELXS-97 (Sheldrick, 1997)
 SHELXTL (Sheldrick, 2000)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 1994)
;
_computing_publication_material      'PLATON (Spek, 2003)'

#===============================================================================

# 8. REFINEMENT DATA


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
```

```
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1052P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?
_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          10263
_refine_ls_number_parameters      713
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.1502
_refine_ls_R_factor_gt            0.0679
_refine_ls_wR_factor_ref          0.1921
_refine_ls_wR_factor_gt           0.1614
_refine_ls_goodness_of_fit_ref    0.939
_refine_ls_restrained_S_all       0.939
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.180
_refine_diff_density_min         -0.255
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_vrn_publ_code_void_volume          0.0
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_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
O11 O Uani 0.0040(2) 0.13569(15) 0.52589(8) 1.000 0.0782(10) . .
O12 O Uani -0.2474(3) 0.05765(18) 0.33173(9) 1.000 0.0998(12) . .
O13 O Uani 0.4564(2) 0.34791(17) 0.41784(9) 1.000 0.0870(11) . .
O14 O Uani 0.49246(19) 0.31203(15) 0.34429(8) 1.000 0.0648(9) . .
N11 N Uani 0.3032(2) 0.32651(15) 0.36727(8) 1.000 0.0502(10) . .
C11 C Uani -0.0538(4) 0.1005(3) 0.56402(13) 1.000 0.104(2) . .
```

```
C12 C Uani -0.0439(3) 0.1250(2) 0.48313(12) 1.000 0.0593(12) . .
C13 C Uani -0.1540(3) 0.0909(2) 0.47342(13) 1.000 0.0696(16) . .
C14 C Uani -0.1895(3) 0.0787(2) 0.42841(14) 1.000 0.0708(16) . .
C15 C Uani -0.1178(3) 0.09938(19) 0.39253(12) 1.000 0.0588(12) . .
C16 C Uani -0.1448(4) 0.0739(2) 0.34484(13) 1.000 0.0650(16) . .
C17 C Uani -0.0426(4) 0.06522(19) 0.31450(12) 1.000 0.0633(14) . .
C18 C Uani -0.0466(5) 0.0130(2) 0.27709(14) 1.000 0.0815(18) . .
C19 C Uani 0.0495(5) 0.0037(3) 0.24950(16) 1.000 0.0959(19) . .
C110 C Uani 0.1522(4) 0.0475(2) 0.25769(13) 1.000 0.0830(17) . .
C111 C Uani 0.1573(3) 0.10062(19) 0.29424(11) 1.000 0.0612(14) . .
C112 C Uani 0.0610(3) 0.11016(18) 0.32296(11) 1.000 0.0529(11) . .
C113 C Uani 0.0574(3) 0.16931(18) 0.36154(10) 1.000 0.0489(11) . .
C114 C Uani -0.0098(3) 0.13990(17) 0.40193(11) 1.000 0.0490(11) . .
C115 C Uani 0.0258(3) 0.15121(18) 0.44719(11) 1.000 0.0530(12) . .
C116 C Uani 0.0968(3) 0.24468(17) 0.35731(10) 1.000 0.0430(11) . .
C117 C Uani 0.1505(3) 0.27794(17) 0.31527(10) 1.000 0.0439(11) . .
C118 C Uani 0.0922(3) 0.27786(17) 0.27100(10) 1.000 0.0446(11) . .
C119 C Uani -0.0253(3) 0.24766(18) 0.26308(11) 1.000 0.0527(12) . .
C120 C Uani -0.0738(3) 0.2443(2) 0.22016(12) 1.000 0.0639(14) . .
C121 C Uani -0.0097(3) 0.2712(2) 0.18213(13) 1.000 0.0715(16) . .
C122 C Uani 0.1000(3) 0.3042(2) 0.18852(11) 1.000 0.0667(16) . .
C123 C Uani 0.1526(3) 0.30953(18) 0.23287(10) 1.000 0.0486(12) . .
C124 C Uani 0.2632(3) 0.3469(2) 0.24068(12) 1.000 0.0603(12) . .
C125 C Uani 0.3112(3) 0.35571(19) 0.28377(11) 1.000 0.0543(12) . .
C126 C Uani 0.2562(3) 0.31955(18) 0.32152(10) 1.000 0.0466(11) . .
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C128 C Uani 0.0941(3) 0.30833(17) 0.39400(10) 1.000 0.0497(11) . .
C129 C Uani 0.0219(3) 0.38114(19) 0.37796(13) 1.000 0.0688(14) . .
C130 C Uani 0.4223(3) 0.3316(2) 0.37945(12) 1.000 0.0597(12) . .
C131 C Uani 0.6222(3) 0.3287(3) 0.34635(13) 1.000 0.0710(14) . .
C132 C Uani 0.6593(4) 0.3037(3) 0.29851(14) 1.000 0.115(2) . .
C133 C Uani 0.6400(4) 0.4170(3) 0.35399(19) 1.000 0.124(3) . .
C134 C Uani 0.6827(3) 0.2776(3) 0.38249(13) 1.000 0.0943(19) . .


H11 H Uiso -0.13198 0.12249 0.56667 1.000 0.1554 . .
H11' H Uiso -0.00858 0.11105 0.59159 1.000 0.1554 . .
H11" H Uiso -0.05953 0.04418 0.55945 1.000 0.1554 . .
H13 H Uiso -0.20357 0.07630 0.49716 1.000 0.0830 . .
H14 H Uiso -0.26343 0.05608 0.42217 1.000 0.0850 . .
H18 H Uiso -0.11555 -0.01584 0.27093 1.000 0.0977 . .
H19 H Uiso 0.04604 -0.03199 0.22520 1.000 0.1150 . .
H110 H Uiso 0.21725 0.04139 0.23883 1.000 0.0994 . .
H111 H Uiso 0.22602 0.13011 0.29953 1.000 0.0729 . .
H115 H Uiso 0.09745 0.17674 0.45368 1.000 0.0634 . .
H119 H Uiso -0.06914 0.23003 0.28780 1.000 0.0636 . .
H120 H Uiso -0.15001 0.22403 0.21582 1.000 0.0767 . .
H121 H Uiso -0.04220 0.26637 0.15271 1.000 0.0854 . .
H122 H Uiso 0.14073 0.32348 0.16340 1.000 0.0801 . .
H124 H Uiso 0.30470 0.36617 0.21575 1.000 0.0723 . .
H125 H Uiso 0.38003 0.38549 0.28821 1.000 0.0651 . .
H127 H Uiso 0.22557 0.38118 0.42057 1.000 0.0738 . .
H127' H Uiso 0.25150 0.29121 0.43000 1.000 0.0738 . .
H128 H Uiso 0.05593 0.28609 0.42107 1.000 0.0595 . .
H129 H Uiso 0.06177 0.40660 0.35315 1.000 0.1032 . .
H129' H Uiso 0.01455 0.41774 0.40298 1.000 0.1032 . .
H129" H Uiso -0.05579 0.36447 0.36777 1.000 0.1032 . .
H132 H Uiso 0.65522 0.24700 0.29594 1.000 0.1723 . .
H132' H Uiso 0.73925 0.32098 0.29336 1.000 0.1723 . .
H132" H Uiso 0.60690 0.32744 0.27607 1.000 0.1723 . .
H133 H Uiso 0.59766 0.44611 0.33058 1.000 0.1858 . .
H133' H Uiso 0.72316 0.42938 0.35270 1.000 0.1858 . .
H133" H Uiso 0.61057 0.43149 0.38352 1.000 0.1858 . .
H134 H Uiso 0.65773 0.29398 0.41235 1.000 0.1413 . .
H134' H Uiso 0.76724 0.28344 0.38046 1.000 0.1413 . .
H134" H Uiso 0.66137 0.22310 0.37759 1.000 0.1413 . .
```

```
O21 O Uani 0.4880(2) 0.37096(16) -0.08980(8) 1.000 0.0820(10) . .
O22 O Uani 0.2734(2) 0.40018(15) 0.11089(8) 1.000 0.0716(10) . .
O23 O Uani 0.9723(2) 0.15133(16) -0.00440(8) 1.000 0.0727(10) . .
O24 O Uani 1.01507(19) 0.13847(14) 0.07196(7) 1.000 0.0643(9) . .
N21 N Uani 0.8233(2) 0.14716(15) 0.04663(8) 1.000 0.0494(10) . .
C21 C Uani 0.4055(4) 0.3899(3) -0.12621(12) 1.000 0.095(2) . .
C22 C Uani 0.4495(3) 0.3726(2) -0.04602(11) 1.000 0.0601(14) . .
C23 C Uani 0.3416(3) 0.4026(2) -0.03240(13) 1.000 0.0639(12) . .
C24 C Uani 0.3150(3) 0.40400(19) 0.01347(12) 1.000 0.0591(12) . .
C25 C Uani 0.3949(3) 0.37426(17) 0.04636(11) 1.000 0.0464(11) . .
C26 C Uani 0.3731(3) 0.38649(18) 0.09545(11) 1.000 0.0519(11) . .
C27 C Uani 0.4811(3) 0.38697(17) 0.12589(10) 1.000 0.0444(11) . .
C28 C Uani 0.4838(3) 0.43017(18) 0.16660(11) 1.000 0.0552(12) . .
C29 C Uani 0.5862(3) 0.4318(2) 0.19365(11) 1.000 0.0620(14) . .
C210 C Uani 0.6859(3) 0.3900(2) 0.18071(11) 1.000 0.0581(12) . .
C211 C Uani 0.6836(3) 0.34602(18) 0.14057(10) 1.000 0.0498(11) . .
C212 C Uani 0.5818(3) 0.34345(17) 0.11211(10) 1.000 0.0444(11) . .
C213 C Uani 0.5744(3) 0.29771(17) 0.06872(9) 1.000 0.0413(10) . .
C214 C Uani 0.5007(3) 0.33803(17) 0.03256(10) 1.000 0.0438(11) . .
C215 C Uani 0.5288(3) 0.33992(19) -0.01373(11) 1.000 0.0541(12) . .
C216 C Uani 0.6140(3) 0.22162(17) 0.06515(9) 1.000 0.0412(10) . .
C217 C Uani 0.6711(3) 0.17438(17) 0.10237(10) 1.000 0.0428(11) . .
C218 C Uani 0.6136(3) 0.15566(17) 0.14475(10) 1.000 0.0446(11) . .
C219 C Uani 0.4985(3) 0.18460(19) 0.15620(12) 1.000 0.0566(12) . .
C220 C Uani 0.4480(3) 0.1686(2) 0.19698(12) 1.000 0.0654(12) . .
C221 C Uani 0.5098(4) 0.1225(2) 0.22970(13) 1.000 0.0774(16) . .
C222 C Uani 0.6176(4) 0.0904(2) 0.21988(12) 1.000 0.0717(16) . .
C223 C Uani 0.6712(3) 0.10504(18) 0.17727(10) 1.000 0.0507(11) . .
C224 C Uani 0.7794(3) 0.0690(2) 0.16479(12) 1.000 0.0594(12) . .
C225 C Uani 0.8297(3) 0.08167(19) 0.12340(11) 1.000 0.0577(12) . .
C226 C Uani 0.7758(3) 0.13541(17) 0.09152(10) 1.000 0.0442(11) . .
C227 C Uani 0.7423(3) 0.1653(2) 0.00733(10) 1.000 0.0553(11) . .
C228 C Uani 0.6125(3) 0.17171(18) 0.02155(10) 1.000 0.0495(11) . .
C229 C Uani 0.5520(3) 0.0913(2) 0.02711(12) 1.000 0.0725(16) . .
C230 C Uani 0.9423(3) 0.1458(2) 0.03499(12) 1.000 0.0580(12) . .
C231 C Uani 1.1442(3) 0.1263(2) 0.06617(12) 1.000 0.0593(14) . .
C232 C Uani 1.1995(3) 0.2009(2) 0.04699(15) 1.000 0.0917(19) . .
C233 C Uani 1.1667(3) 0.0546(2) 0.03615(14) 1.000 0.0826(17) . .
C234 C Uani 1.1854(3) 0.1106(3) 0.11501(14) 1.000 0.0923(19) . .


H21 H Uiso 0.33632 0.35686 -0.12386 1.000 0.1430 . .
H21' H Uiso 0.44217 0.38084 -0.15520 1.000 0.1430 . .
H21" H Uiso 0.38260 0.44459 -0.12394 1.000 0.1430 . .
H23 H Uiso 0.28713 0.42166 -0.05409 1.000 0.0765 . .
H24 H Uiso 0.24289 0.42506 0.02268 1.000 0.0708 . .
H28 H Uiso 0.41682 0.45797 0.17562 1.000 0.0659 . .
H29 H Uiso 0.58787 0.46110 0.22067 1.000 0.0742 . .
H210 H Uiso 0.75453 0.39151 0.19895 1.000 0.0696 . .
H211 H Uiso 0.75078 0.31763 0.13235 1.000 0.0599 . .
H215 H Uiso 0.60085 0.31926 -0.02325 1.000 0.0645 . .
H219 H Uiso 0.45689 0.21549 0.13492 1.000 0.0679 . .
H220 H Uiso 0.37266 0.18804 0.20329 1.000 0.0784 . .
H221 H Uiso 0.47698 0.11383 0.25830 1.000 0.0930 . .
H222 H Uiso 0.65628 0.05842 0.24146 1.000 0.0857 . .
H224 H Uiso 0.81752 0.03545 0.18566 1.000 0.0711 . .
H225 H Uiso 0.89921 0.05526 0.11588 1.000 0.0692 . .
H227 H Uiso 0.74925 0.12384 -0.01556 1.000 0.0662 . .
H227' H Uiso 0.76637 0.21488 -0.00656 1.000 0.0662 . .
H228 H Uiso 0.56912 0.20130 -0.00234 1.000 0.0593 . .
H229 H Uiso 0.59909 0.05854 0.04734 1.000 0.1088 . .
H229' H Uiso 0.54424 0.06597 -0.00228 1.000 0.1088 . .
H229" H Uiso 0.47470 0.09878 0.03977 1.000 0.1088 . .
H232 H Uiso 1.16868 0.21015 0.01655 1.000 0.1374 . .
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H232' H Uiso 1.28414 0.19454 0.04605 1.000 0.1374 . .
H232" H Uiso 1.18060 0.24517 0.06622 1.000 0.1374 . .
H233 H Uiso 1.11852 0.01109 0.04607 1.000 0.1236 . .
H233' H Uiso 1.24905 0.04007 0.03852 1.000 0.1236 . .
H233" H Uiso 1.14679 0.06729 0.00485 1.000 0.1236 . .
H234 H Uiso 1.16521 0.15500 0.13394 1.000 0.1380 . .
H234' H Uiso 1.26997 0.10309 0.11583 1.000 0.1380 . .
H234" H Uiso 1.14721 0.06370 0.12624 1.000 0.1380 . .


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_atom_site_aniso_U_22
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_atom_site_aniso_U_12
O11 0.0901(19) 0.0915(19) 0.0531(16) 0.0002(13) 0.0057(14) -0.0193(15)
O12 0.087(2) 0.119(2) 0.092(2) 0.0335(17) -0.0375(17) -0.0521(18)
O13 0.0665(18) 0.134(2) 0.0603(17) -0.0215(16) -0.0079(14) -0.0231(16)
O14 0.0392(14) 0.1011(19) 0.0539(15) 0.0008(13) -0.0005(11) -0.0043(12)
N11 0.0425(16) 0.0664(18) 0.0418(16) -0.0049(13) 0.0031(13) -0.0090(13)
C11 0.125(4) 0.132(4) 0.055(3) 0.002(3) 0.024(3) -0.023(3)
C12 0.062(2) 0.057(2) 0.059(2) 0.0034(18) 0.0002(19) -0.0090(18)
C13 0.065(3) 0.071(2) 0.073(3) 0.015(2) 0.011(2) -0.017(2)
C14 0.056(2) 0.075(3) 0.081(3) 0.019(2) -0.010(2) -0.0184(19)
C15 0.055(2) 0.054(2) 0.067(2) 0.0223(18) -0.0106(19) -0.0174(17)
C16 0.069(3) 0.055(2) 0.070(3) 0.0231(18) -0.028(2) -0.0231(19)
C17 0.083(3) 0.045(2) 0.061(2) 0.0096(18) -0.026(2) -0.0074(19)
C18 0.113(4) 0.057(2) 0.073(3) -0.002(2) -0.040(3) -0.008(2)
C19 0.133(4) 0.073(3) 0.080(3) -0.027(2) -0.046(3) 0.022(3)
C110 0.101(3) 0.082(3) 0.065(3) -0.018(2) -0.024(2) 0.035(3)
C111 0.075(3) 0.053(2) 0.055(2) -0.0082(17) -0.018(2) 0.0132(18)
C112 0.063(2) 0.0462(19) 0.049(2) -0.0004(16) -0.0158(18) -0.0003(17)
C113 0.054(2) 0.0444(19) 0.048(2) 0.0033(15) -0.0076(16) -0.0037(15)
C114 0.049(2) 0.0456(19) 0.052(2) 0.0073(15) -0.0055(16) -0.0070(15)
C115 0.052(2) 0.050(2) 0.057(2) 0.0039(16) 0.0029(18) -0.0080(16)
C116 0.0414(18) 0.0443(19) 0.0431(19) -0.0018(14) -0.0008(14) -0.0064(14)
C117 0.0449(19) 0.0433(17) 0.0436(19) -0.0001(14) 0.0039(15) 0.0001(15)
C118 0.0419(19) 0.0430(17) 0.049(2) -0.0027(15) 0.0005(16) 0.0057(14)
C119 0.043(2) 0.053(2) 0.062(2) 0.0061(16) -0.0053(17) 0.0028(15)
C120 0.055(2) 0.068(2) 0.068(3) 0.0045(19) -0.017(2) 0.0008(18)
C121 0.064(3) 0.090(3) 0.060(2) 0.001(2) -0.015(2) 0.002(2)
C122 0.066(3) 0.088(3) 0.046(2) 0.0016(19) 0.0020(19) 0.016(2)
C123 0.045(2) 0.054(2) 0.047(2) 0.0013(15) 0.0033(16) 0.0073(16)
C124 0.046(2) 0.080(2) 0.055(2) 0.0139(19) 0.0069(18) -0.0006(18)
C125 0.041(2) 0.065(2) 0.057(2) 0.0079(17) 0.0041(17) -0.0030(16)
C126 0.0440(19) 0.0506(19) 0.0454(19) -0.0004(15) 0.0045(16) -0.0044(15)
C127 0.055(2) 0.074(2) 0.057(2) -0.0146(18) 0.0111(18) -0.0111(18)
C128 0.052(2) 0.0455(19) 0.052(2) -0.0042(15) 0.0141(16) -0.0092(15)
C129 0.067(2) 0.050(2) 0.090(3) -0.0033(19) 0.020(2) -0.0011(18)
C130 0.051(2) 0.078(2) 0.050(2) -0.0022(19) -0.003(2) -0.0118(19)
C131 0.039(2) 0.109(3) 0.065(2) 0.024(2) -0.0026(18) -0.011(2)
C132 0.060(3) 0.206(6) 0.079(3) 0.015(3) 0.014(2) 0.020(3)
C133 0.072(3) 0.097(4) 0.203(6) 0.021(4) 0.007(3) -0.032(3)
C134 0.061(3) 0.130(4) 0.091(3) 0.033(3) -0.022(2) -0.008(2)
O21 0.0790(18) 0.118(2) 0.0487(16) 0.0167(14) -0.0089(13) 0.0140(16)
O22 0.0486(16) 0.0892(18) 0.0775(17) -0.0013(14) 0.0139(13) 0.0143(13)
O23 0.0627(17) 0.102(2) 0.0539(16) 0.0040(14) 0.0132(13) 0.0091(14)
O24 0.0425(14) 0.0920(18) 0.0585(15) -0.0025(12) 0.0007(12) 0.0118(12)
N21 0.0431(17) 0.0622(17) 0.0431(16) -0.0016(12) 0.0028(13) 0.0126(13)
C21 0.112(4) 0.114(4) 0.059(3) 0.030(2) -0.030(2) -0.008(3)
C22 0.068(3) 0.069(2) 0.043(2) 0.0098(17) -0.0050(19) 0.0028(19)
C23 0.060(2) 0.069(2) 0.062(2) 0.0069(19) -0.0147(19) 0.0138(19)
C24 0.052(2) 0.061(2) 0.064(2) 0.0051(18) -0.0070(18) 0.0123(17)
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```
C25 0.0418(19) 0.0431(18) 0.054(2) 0.0027(15) -0.0030(16) 0.0045(14)
C26 0.050(2) 0.0451(19) 0.061(2) 0.0006(16) 0.0096(18) 0.0064(16)
C27 0.047(2) 0.0417(17) 0.0446(19) 0.0008(14) 0.0078(15) 0.0041(14)
C28 0.061(2) 0.051(2) 0.054(2) -0.0050(16) 0.0137(18) 0.0088(16)
C29 0.085(3) 0.055(2) 0.046(2) -0.0087(16) 0.001(2) 0.0044(19)
C210 0.065(2) 0.062(2) 0.047(2) -0.0024(17) -0.0037(18) -0.0013(19)
C211 0.054(2) 0.0489(19) 0.0465(19) -0.0007(16) -0.0014(16) 0.0032(15)
C212 0.050(2) 0.0426(17) 0.0408(18) 0.0032(14) 0.0035(16) 0.0031(15)
C213 0.0412(18) 0.0470(18) 0.0355(17) -0.0008(14) -0.0032(14) 0.0041(14)
C214 0.0427(19) 0.0468(18) 0.0418(19) 0.0009(14) -0.0015(15) 0.0066(15)
C215 0.050(2) 0.062(2) 0.050(2) 0.0060(16) -0.0056(17) 0.0083(16)
C216 0.0412(18) 0.0483(18) 0.0339(17) -0.0023(14) -0.0023(13) 0.0061(14)
C217 0.0430(19) 0.0453(18) 0.0399(18) -0.0027(14) -0.0039(15) 0.0069(14)
C218 0.045(2) 0.0475(18) 0.0412(18) -0.0036(15) 0.0004(15) 0.0013(15)
C219 0.053(2) 0.056(2) 0.061(2) 0.0027(17) 0.0045(18) 0.0033(17)
C220 0.061(2) 0.071(2) 0.065(2) 0.006(2) 0.023(2) 0.0018(19)
C221 0.088(3) 0.090(3) 0.055(2) 0.005(2) 0.020(2) -0.003(2)
C222 0.080(3) 0.077(3) 0.058(2) 0.016(2) -0.002(2) 0.001(2)
C223 0.059(2) 0.0510(19) 0.042(2) 0.0046(16) -0.0020(17) 0.0015(17)
C224 0.062(2) 0.061(2) 0.055(2) 0.0168(17) -0.0041(19) 0.0115(18)
C225 0.053(2) 0.061(2) 0.059(2) 0.0113(18) 0.0012(18) 0.0165(16)
C226 0.0443(19) 0.0497(18) 0.0385(18) -0.0011(14) -0.0017(15) 0.0052(15)
C227 0.057(2) 0.067(2) 0.0417(19) -0.0057(16) -0.0030(16) 0.0159(17)
C228 0.049(2) 0.054(2) 0.0451(19) -0.0086(15) -0.0094(15) 0.0093(16)
C229 0.073(3) 0.066(2) 0.078(3) -0.015(2) -0.014(2) 0.000(2)
C230 0.055(2) 0.068(2) 0.051(2) -0.0037(18) 0.004(2) 0.0062(17)
C231 0.038(2) 0.059(2) 0.081(3) 0.0004(19) 0.0078(18) 0.0038(16)
C232 0.070(3) 0.071(3) 0.134(4) 0.002(3) 0.002(3) -0.004(2)
C233 0.061(3) 0.072(3) 0.115(3) -0.008(2) 0.010(2) 0.012(2)
C234 0.059(3) 0.121(4) 0.096(3) 0.000(3) -0.019(2) 0.017(2)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 O11     C11        1.428(5)                    .      .                   yes
 O11     C12        1.361(4)                    .      .                   yes
 O12     C16        1.240(5)                    .      .                   yes
 O13     C130       1.209(4)                    .      .                   yes
 O14     C130       1.347(4)                    .      .                   yes
 O14     C131       1.487(4)                    .      .                   yes
 O21     C22        1.356(4)                    .      .                   yes
 O21     C21        1.434(5)                    .      .                   yes
 O22     C26        1.239(4)                    .      .                   yes
 O23     C230       1.207(4)                    .      .                   yes
 O24     C231       1.481(4)                    .      .                   yes
 O24     C230       1.348(4)                    .      .                   yes
 N11     C127       1.483(4)                    .      .                   yes
 N11     C126       1.431(4)                    .      .                   yes
 N11     C130       1.383(4)                    .      .                   yes
```

N21	C226	1.437(4)	.	.	yes
N21	C227	1.483(4)	.	.	yes
N21	C230	1.388(4)	.	.	yes
C12	C13	1.390(5)	.	.	no
C12	C115	1.393(5)	.	.	no
C13	C14	1.380(5)	.	.	no
C14	C15	1.378(5)	.	.	no
C15	C114	1.417(5)	.	.	no
C15	C16	1.482(5)	.	.	no
C16	C17	1.471(6)	.	.	no
C17	C112	1.408(5)	.	.	no
C17	C18	1.402(5)	.	.	no
C18	C19	1.369(7)	.	.	no
C19	C110	1.389(7)	.	.	no
C110	C111	1.392(5)	.	.	no
C111	C112	1.391(5)	.	.	no
C11	H11	0.9593	.	.	no
C11	H11"	0.9605	.	.	no
C11	H11'	0.9602	.	.	no
C112	C113	1.504(4)	.	.	no
C13	H13	0.9303	.	.	no
C113	C114	1.496(4)	.	.	no
C113	C116	1.352(4)	.	.	no
C14	H14	0.9302	.	.	no
C114	C115	1.385(5)	.	.	no
C116	C117	1.487(4)	.	.	no
C116	C128	1.516(4)	.	.	no
C117	C118	1.437(4)	.	.	no
C117	C126	1.390(5)	.	.	no
C18	H18	0.9304	.	.	no
C118	C119	1.432(5)	.	.	no
C118	C123	1.418(4)	.	.	no
C119	C120	1.357(5)	.	.	no
C19	H19	0.9298	.	.	no
C120	C121	1.409(5)	.	.	no
C121	C122	1.364(5)	.	.	no
C122	C123	1.415(4)	.	.	no
C123	C124	1.410(5)	.	.	no
C124	C125	1.367(5)	.	.	no
C125	C126	1.411(4)	.	.	no
C127	C128	1.532(5)	.	.	no
C128	C129	1.540(4)	.	.	no
C131	C134	1.513(6)	.	.	no
C131	C132	1.523(6)	.	.	no
C131	C133	1.518(7)	.	.	no
C110	H110	0.9295	.	.	no
C111	H111	0.9299	.	.	no
C115	H115	0.9304	.	.	no
C119	H119	0.9298	.	.	no
C120	H120	0.9298	.	.	no
C121	H121	0.9300	.	.	no
C22	C215	1.399(5)	.	.	no
C122	H122	0.9299	.	.	no
C22	C23	1.381(5)	.	.	no
C23	C24	1.376(5)	.	.	no
C124	H124	0.9299	.	.	no
C24	C25	1.396(5)	.	.	no
C125	H125	0.9302	.	.	no
C25	C26	1.471(5)	.	.	no
C25	C214	1.404(5)	.	.	no
C26	C27	1.492(5)	.	.	no
C127	H127	0.9703	.	.	no
C27	C28	1.393(4)	.	.	no
C27	C212	1.415(5)	.	.	no
C127	H127'	0.9697	.	.	no
C28	C29	1.385(5)	.	.	no

C128	H128	0.9802	.	.	no
C129	H129"	0.9604	.	.	no
C129	H129	0.9597	.	.	no
C129	H129'	0.9602	.	.	no
C29	C210	1.383(5)	.	.	no
C132	H132"	0.9602	.	.	no
C132	H132'	0.9603	.	.	no
C132	H132	0.9596	.	.	no
C133	H133"	0.9599	.	.	no
C133	H133	0.9601	.	.	no
C133	H133'	0.9604	.	.	no
C134	H134"	0.9594	.	.	no
C134	H134	0.9605	.	.	no
C134	H134'	0.9595	.	.	no
C21	H21"	0.9597	.	.	no
C21	H21'	0.9598	.	.	no
C21	H21	0.9608	.	.	no
C23	H23	0.9300	.	.	no
C24	H24	0.9300	.	.	no
C28	H28	0.9297	.	.	no
C29	H29	0.9298	.	.	no
C210	C211	1.385(4)	.	.	no
C211	C212	1.403(5)	.	.	no
C212	C213	1.483(4)	.	.	no
C213	C214	1.493(4)	.	.	no
C213	C216	1.362(4)	.	.	no
C214	C215	1.393(4)	.	.	no
C216	C217	1.483(4)	.	.	no
C216	C228	1.524(4)	.	.	no
C217	C218	1.441(4)	.	.	no
C217	C226	1.391(5)	.	.	no
C218	C223	1.423(4)	.	.	no
C218	C219	1.430(5)	.	.	no
C219	C220	1.355(5)	.	.	no
C220	C221	1.405(5)	.	.	no
C221	C222	1.364(6)	.	.	no
C222	C223	1.413(5)	.	.	no
C223	C224	1.415(5)	.	.	no
C224	C225	1.360(5)	.	.	no
C225	C226	1.426(4)	.	.	no
C227	C228	1.530(5)	.	.	no
C228	C229	1.527(5)	.	.	no
C231	C232	1.515(5)	.	.	no
C231	C233	1.516(5)	.	.	no
C231	C234	1.513(5)	.	.	no
C210	H210	0.9301	.	.	no
C211	H211	0.9300	.	.	no
C215	H215	0.9297	.	.	no
C219	H219	0.9299	.	.	no
C220	H220	0.9306	.	.	no
C221	H221	0.9299	.	.	no
C222	H222	0.9306	.	.	no
C224	H224	0.9298	.	.	no
C225	H225	0.9299	.	.	no
C227	H227'	0.9694	.	.	no
C227	H227	0.9705	.	.	no
C228	H228	0.9798	.	.	no
C229	H229'	0.9600	.	.	no
C229	H229"	0.9597	.	.	no
C229	H229	0.9604	.	.	no
C232	H232'	0.9596	.	.	no
C232	H232"	0.9596	.	.	no
C232	H232	0.9598	.	.	no
C233	H233'	0.9600	.	.	no
C233	H233"	0.9600	.	.	no
C233	H233	0.9599	.	.	no

```
 C234    H234'        0.9601                    .       .                 no
 C234    H234"        0.9602                    .       .                 no
 C234    H234         0.9597                    .       .                 no

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_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 C11     O11     C12        118.7(3)              .       .       .         yes
 C130    O14     C131       120.8(3)              .       .       .         yes
 C21     O21     C22        118.6(3)              .       .       .         yes
 C230    O24     C231       120.3(2)              .       .       .         yes
 C126    N11     C130       125.8(3)              .       .       .         yes
 C126    N11     C127       120.7(2)              .       .       .         yes
 C127    N11     C130       113.5(2)              .       .       .         yes
 C226    N21     C230       126.7(3)              .       .       .         yes
 C227    N21     C230       113.4(2)              .       .       .         yes
 C226    N21     C227       119.9(2)              .       .       .         yes
 O11     C12     C115       115.4(3)              .       .       .         yes
 C13     C12     C115       119.4(3)              .       .       .         no
 O11     C12     C13        125.3(3)              .       .       .         yes
 C12     C13     C14        119.8(3)              .       .       .         no
 C13     C14     C15        121.4(3)              .       .       .         no
 C16     C15     C114       118.8(3)              .       .       .         no
 C14     C15     C16        121.8(3)              .       .       .         no
 C14     C15     C114       119.2(3)              .       .       .         no
 O12     C16     C17        121.8(3)              .       .       .         yes
 O12     C16     C15        121.8(4)              .       .       .         yes
 C15     C16     C17        116.4(4)              .       .       .         no
 C16     C17     C18        121.1(4)              .       .       .         no
 C16     C17     C112       119.7(3)              .       .       .         no
 C18     C17     C112       119.3(4)              .       .       .         no
 C17     C18     C19        121.0(5)              .       .       .         no
 C18     C19     C110       120.2(4)              .       .       .         no
 C19     C110    C111       119.7(4)              .       .       .         no
 H11'    C11     H11"         109.41              .       .       .         no
 H11     C11     H11"         109.49              .       .       .         no
 O11     C11     H11          109.52              .       .       .         no
 C110    C111    C112       120.9(3)              .       .       .         no
 H11     C11     H11'         109.50              .       .       .         no
 O11     C11     H11'         109.46              .       .       .         no
 O11     C11     H11"         109.44              .       .       .         no
 C17     C112    C111       119.0(3)              .       .       .         no
 C111    C112    C113       124.0(3)              .       .       .         no
 C17     C112    C113       117.0(3)              .       .       .         no
 C14     C13     H13          120.08              .       .       .         no
 C114    C113    C116       123.7(3)              .       .       .         no
 C112    C113    C114       113.0(3)              .       .       .         no
 C12     C13     H13          120.15              .       .       .         no
 C112    C113    C116       122.8(3)              .       .       .         no
 C113    C114    C115       124.3(3)              .       .       .         no
 C15     C14     H14          119.30              .       .       .         no
 C15     C114    C115       118.9(3)              .       .       .         no
 C13     C14     H14          119.29              .       .       .         no
 C15     C114    C113       116.9(3)              .       .       .         no
 C12     C115    C114       121.1(3)              .       .       .         no
 C117    C116    C128       109.2(2)              .       .       .         no
 C113    C116    C117       124.7(3)              .       .       .         no
 C113    C116    C128       126.1(3)              .       .       .         no
 C116    C117    C126       116.2(3)              .       .       .         no
 C116    C117    C118       123.7(3)              .       .       .         no
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C118	C117	C126	119.6(3)	.	.	.	no
C19	C18	H18	119.47	.	.	.	no
C117	C118	C123	119.1(3)	.	.	.	no
C17	C18	H18	119.54	.	.	.	no
C117	C118	C119	123.4(3)	.	.	.	no
C119	C118	C123	117.5(3)	.	.	.	no
C18	C19	H19	119.97	.	.	.	no
C110	C19	H19	119.87	.	.	.	no
C118	C119	C120	121.2(3)	.	.	.	no
C119	C120	C121	120.6(3)	.	.	.	no
C120	C121	C122	119.9(3)	.	.	.	no
C121	C122	C123	120.9(3)	.	.	.	no
C118	C123	C122	119.6(3)	.	.	.	no
C122	C123	C124	122.0(3)	.	.	.	no
C118	C123	C124	118.4(3)	.	.	.	no
C123	C124	C125	122.0(3)	.	.	.	no
C124	C125	C126	119.9(3)	.	.	.	no
N11	C126	C117	117.7(3)	.	.	.	yes
C117	C126	C125	120.2(3)	.	.	.	no
N11	C126	C125	122.1(3)	.	.	.	yes
N11	C127	C128	112.8(2)	.	.	.	yes
C127	C128	C129	113.0(3)	.	.	.	no
C116	C128	C127	107.6(3)	.	.	.	no
C116	C128	C129	111.5(3)	.	.	.	no
O14	C130	N11	111.6(3)	.	.	.	yes
O13	C130	N11	122.8(3)	.	.	.	yes
O13	C130	O14	125.5(3)	.	.	.	yes
O14	C131	C133	108.6(3)	.	.	.	yes
C133	C131	C134	113.5(4)	.	.	.	no
O14	C131	C132	101.3(3)	.	.	.	yes
C132	C131	C133	111.6(4)	.	.	.	no
C132	C131	C134	110.7(4)	.	.	.	no
O14	C131	C134	110.5(3)	.	.	.	yes
C111	C110	H110	120.16	.	.	.	no
C19	C110	H110	120.11	.	.	.	no
C112	C111	H111	119.55	.	.	.	no
C110	C111	H111	119.54	.	.	.	no
C12	C115	H115	119.46	.	.	.	no
C114	C115	H115	119.46	.	.	.	no
C118	C119	H119	119.36	.	.	.	no
C120	C119	H119	119.43	.	.	.	no
C119	C120	H120	119.68	.	.	.	no
C121	C120	H120	119.71	.	.	.	no
C122	C121	H121	120.10	.	.	.	no
C120	C121	H121	119.97	.	.	.	no
O21	C22	C23	125.2(3)	.	.	.	yes
O21	C22	C215	114.5(3)	.	.	.	yes
C121	C122	H122	119.54	.	.	.	no
C123	C122	H122	119.58	.	.	.	no
C23	C22	C215	120.3(3)	.	.	.	no
C22	C23	C24	119.6(3)	.	.	.	no
C125	C124	H124	119.02	.	.	.	no
C123	C124	H124	118.98	.	.	.	no
C23	C24	C25	120.9(3)	.	.	.	no
C124	C125	H125	120.05	.	.	.	no
C126	C125	H125	120.04	.	.	.	no
C26	C25	C214	119.8(3)	.	.	.	no
C24	C25	C26	120.1(3)	.	.	.	no
C24	C25	C214	119.9(3)	.	.	.	no
O22	C26	C27	121.1(3)	.	.	.	yes
O22	C26	C25	123.3(3)	.	.	.	yes
C25	C26	C27	115.5(3)	.	.	.	no
N11	C127	H127'	109.03	.	.	.	no
C26	C27	C28	121.0(3)	.	.	.	no
C26	C27	C212	118.5(3)	.	.	.	no
C28	C27	C212	120.6(3)	.	.	.	no

H127'	C127	H127	107.80	.	.	.	no
C128	C127	H127	109.01	.	.	.	no
N11	C127	H127	109.01	.	.	.	no
C128	C127	H127'	109.04	.	.	.	no
C116	C128	H128	108.22	.	.	.	no
C127	C128	H128	108.22	.	.	.	no
C129	C128	H128	108.22	.	.	.	no
C27	C28	C29	120.1(3)	.	.	.	no
C128	C129	H129'	109.48	.	.	.	no
H129"	C129	H129	109.47	.	.	.	no
C128	C129	H129	109.50	.	.	.	no
H129'	C129	H129"	109.41	.	.	.	no
C128	C129	H129"	109.47	.	.	.	no
C28	C29	C210	120.4(3)	.	.	.	no
H129'	C129	H129	109.49	.	.	.	no
C131	C132	H132"	109.49	.	.	.	no
C131	C132	H132'	109.44	.	.	.	no
C131	C132	H132	109.48	.	.	.	no
H132'	C132	H132"	109.43	.	.	.	no
H132'	C132	H132	109.48	.	.	.	no
H132"	C132	H132	109.50	.	.	.	no
H133'	C133	H133"	109.42	.	.	.	no
H133'	C133	H133	109.42	.	.	.	no
C131	C133	H133	109.53	.	.	.	no
C131	C133	H133'	109.48	.	.	.	no
C131	C133	H133"	109.54	.	.	.	no
H133"	C133	H133	109.44	.	.	.	no
H134"	C134	H134	109.49	.	.	.	no
C131	C134	H134'	109.43	.	.	.	no
C131	C134	H134"	109.45	.	.	.	no
C131	C134	H134	109.41	.	.	.	no
H134'	C134	H134"	109.56	.	.	.	no
H134'	C134	H134	109.48	.	.	.	no
O21	C21	H21	109.44	.	.	.	no
O21	C21	H21'	109.50	.	.	.	no
O21	C21	H21"	109.50	.	.	.	no
H21	C21	H21'	109.44	.	.	.	no
H21	C21	H21"	109.43	.	.	.	no
H21'	C21	H21"	109.51	.	.	.	no
C22	C23	H23	120.21	.	.	.	no
C24	C23	H23	120.17	.	.	.	no
C23	C24	H24	119.59	.	.	.	no
C25	C24	H24	119.56	.	.	.	no
C27	C28	H28	119.98	.	.	.	no
C29	C28	H28	119.97	.	.	.	no
C28	C29	H29	119.79	.	.	.	no
C210	C29	H29	119.86	.	.	.	no
C29	C210	C211	120.0(3)	.	.	.	no
C210	C211	C212	121.2(3)	.	.	.	no
C27	C212	C211	117.8(3)	.	.	.	no
C27	C212	C213	118.6(3)	.	.	.	no
C211	C212	C213	123.6(3)	.	.	.	no
C212	C213	C216	122.8(3)	.	.	.	no
C212	C213	C214	112.8(3)	.	.	.	no
C214	C213	C216	123.6(3)	.	.	.	no
C25	C214	C215	118.5(3)	.	.	.	no
C25	C214	C213	117.3(3)	.	.	.	no
C213	C214	C215	124.2(3)	.	.	.	no
C22	C215	C214	120.5(3)	.	.	.	no
C217	C216	C228	108.2(2)	.	.	.	no
C213	C216	C217	126.0(2)	.	.	.	no
C213	C216	C228	125.8(3)	.	.	.	no
C216	C217	C226	116.4(3)	.	.	.	no
C218	C217	C226	119.2(3)	.	.	.	no
C216	C217	C218	123.4(3)	.	.	.	no
C219	C218	C223	116.9(3)	.	.	.	no

C217	C218	C219	123.3(3)	.	.	.	no
C217	C218	C223	119.8(3)	.	.	.	no
C218	C219	C220	122.3(3)	.	.	.	no
C219	C220	C221	119.7(3)	.	.	.	no
C220	C221	C222	120.5(3)	.	.	.	no
C221	C222	C223	120.8(3)	.	.	.	no
C222	C223	C224	122.3(3)	.	.	.	no
C218	C223	C222	119.6(3)	.	.	.	no
C218	C223	C224	118.0(3)	.	.	.	no
C223	C224	C225	122.4(3)	.	.	.	no
C224	C225	C226	120.0(3)	.	.	.	no
N21	C226	C217	118.3(3)	.	.	.	yes
N21	C226	C225	121.4(3)	.	.	.	yes
C217	C226	C225	120.3(3)	.	.	.	no
N21	C227	C228	112.4(2)	.	.	.	yes
C227	C228	C229	113.3(3)	.	.	.	no
C216	C228	C227	105.6(3)	.	.	.	no
C216	C228	C229	113.5(3)	.	.	.	no
O23	C230	O24	126.3(3)	.	.	.	yes
O23	C230	N21	121.3(3)	.	.	.	yes
O24	C230	N21	112.4(3)	.	.	.	yes
C233	C231	C234	110.6(3)	.	.	.	no
O24	C231	C232	109.8(3)	.	.	.	yes
O24	C231	C233	110.6(3)	.	.	.	yes
O24	C231	C234	101.6(3)	.	.	.	yes
C232	C231	C233	112.0(3)	.	.	.	no
C232	C231	C234	111.8(3)	.	.	.	no
C29	C210	H210	119.96	.	.	.	no
C211	C210	H210	120.02	.	.	.	no
C210	C211	H211	119.37	.	.	.	no
C212	C211	H211	119.39	.	.	.	no
C22	C215	H215	119.73	.	.	.	no
C214	C215	H215	119.73	.	.	.	no
C218	C219	H219	118.85	.	.	.	no
C220	C219	H219	118.88	.	.	.	no
C219	C220	H220	120.14	.	.	.	no
C221	C220	H220	120.13	.	.	.	no
C220	C221	H221	119.75	.	.	.	no
C222	C221	H221	119.71	.	.	.	no
C221	C222	H222	119.65	.	.	.	no
C223	C222	H222	119.59	.	.	.	no
C223	C224	H224	118.80	.	.	.	no
C225	C224	H224	118.81	.	.	.	no
C224	C225	H225	120.01	.	.	.	no
C226	C225	H225	120.01	.	.	.	no
N21	C227	H227'	109.15	.	.	.	no
N21	C227	H227	109.08	.	.	.	no
C228	C227	H227'	109.15	.	.	.	no
C228	C227	H227	109.07	.	.	.	no
H227'	C227	H227	107.85	.	.	.	no
C216	C228	H228	108.05	.	.	.	no
C227	C228	H228	108.00	.	.	.	no
C229	C228	H228	108.06	.	.	.	no
C228	C229	H229'	109.47	.	.	.	no
C228	C229	H229"	109.49	.	.	.	no
C228	C229	H229	109.47	.	.	.	no
H229'	C229	H229"	109.49	.	.	.	no
H229'	C229	H229	109.44	.	.	.	no
H229"	C229	H229	109.46	.	.	.	no
C231	C232	H232'	109.44	.	.	.	no
C231	C232	H232"	109.43	.	.	.	no
C231	C232	H232	109.41	.	.	.	no
H232'	C232	H232"	109.54	.	.	.	no
H232'	C232	H232	109.50	.	.	.	no
H232"	C232	H232	109.51	.	.	.	no
C231	C233	H233'	109.46	.	.	.	no

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 C231    C233    H233"        109.44            .       .       .          no
 C231    C233    H233         109.49            .       .       .          no
 H233'   C233    H233"        109.48            .       .       .          no
 H233'   C233    H233         109.48            .       .       .          no
 H233"   C233    H233         109.48            .       .       .          no
 C231    C234    H234'        109.45            .       .       .          no
 C231    C234    H234"        109.49            .       .       .          no
 C231    C234    H234         109.47            .       .       .          no
 H234'   C234    H234"        109.44            .       .       .          no
 H234'   C234    H234         109.49            .       .       .          no
 H234"   C234    H234         109.48            .       .       .          no

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 C11     O11     C12     C13          8.8(5)     .       .       .       .   no
 C11     O11     C12     C115      -171.3(3)     .       .       .       .   no
 C131    O14     C130    O13        -16.0(5)     .       .       .       .   no
 C131    O14     C130    N11        167.6(3)     .       .       .       .   no
 C130    O14     C131    C132      -175.1(3)     .       .       .       .   no
 C130    O14     C131    C133       -57.5(4)     .       .       .       .   no
 C130    O14     C131    C134        67.6(5)     .       .       .       .   no
 C21     O21     C22     C215       169.1(3)     .       .       .       .   no
 C21     O21     C22     C23        -10.4(5)     .       .       .       .   no
 C230    O24     C231    C232        68.8(4)     .       .       .       .   no
 C230    O24     C231    C234      -172.7(3)     .       .       .       .   no
 C230    O24     C231    C233       -55.3(4)     .       .       .       .   no
 C231    O24     C230    O23         -7.8(5)     .       .       .       .   no
 C231    O24     C230    N21        172.7(3)     .       .       .       .   no
 C130    N11     C126    C117       149.1(3)     .       .       .       .   no
 C126    N11     C127    C128         9.9(4)     .       .       .       .   no
 C130    N11     C127    C128      -169.9(3)     .       .       .       .   no
 C130    N11     C126    C125       -33.3(5)     .       .       .       .   no
 C127    N11     C126    C117       -30.7(4)     .       .       .       .   no
 C126    N11     C130    O14        -13.5(4)     .       .       .       .   no
 C127    N11     C126    C125       146.9(3)     .       .       .       .   no
 C126    N11     C130    O13        169.9(3)     .       .       .       .   no
 C127    N11     C130    O14        166.3(3)     .       .       .       .   no
 C127    N11     C130    O13        -10.3(5)     .       .       .       .   no
 C227    N21     C226    C225       147.4(3)     .       .       .       .   no
 C227    N21     C226    C217       -28.8(4)     .       .       .       .   no
 C227    N21     C230    O23         -6.8(4)     .       .       .       .   no
 C230    N21     C226    C217       149.1(3)     .       .       .       .   no
 C230    N21     C226    C225       -34.7(5)     .       .       .       .   no
 C227    N21     C230    O24        172.7(3)     .       .       .       .   no
 C226    N21     C230    O24         -5.3(4)     .       .       .       .   no
 C230    N21     C227    C228      -176.3(3)     .       .       .       .   no
 C226    N21     C227    C228         1.9(4)     .       .       .       .   no
 C226    N21     C230    O23        175.2(3)     .       .       .       .   no
 O11     C12     C13     C14       -175.9(3)     .       .       .       .   no
 C115    C12     C13     C14          4.2(5)     .       .       .       .   no
 C13     C12     C115    C114        -3.6(5)     .       .       .       .   no
 O11     C12     C115    C114       176.5(3)     .       .       .       .   no
 C12     C13     C14     C15          0.2(5)     .       .       .       .   no
 C13     C14     C15     C114        -5.3(5)     .       .       .       .   no
 C13     C14     C15     C16        168.9(3)     .       .       .       .   no
 C14     C15     C114    C115         5.8(5)     .       .       .       .   no
 C16     C15     C114    C113        12.7(4)     .       .       .       .   no
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C16	C15	C114	C115	-168.6(3)	.	.	.	.	no
C114	C15	C16	C17	22.1(4)	.	.	.	.	no
C114	C15	C16	O12	-160.7(3)	.	.	.	.	no
C14	C15	C16	O12	25.1(5)	.	.	.	.	no
C14	C15	C16	C17	-152.1(3)	.	.	.	.	no
C14	C15	C114	C113	-173.0(3)	.	.	.	.	no
C15	C16	C17	C112	-26.8(5)	.	.	.	.	no
O12	C16	C17	C18	-23.7(5)	.	.	.	.	no
O12	C16	C17	C112	156.1(3)	.	.	.	.	no
C15	C16	C17	C18	153.4(3)	.	.	.	.	no
C18	C17	C112	C111	-0.9(5)	.	.	.	.	no
C16	C17	C112	C111	179.3(3)	.	.	.	.	no
C18	C17	C112	C113	175.9(3)	.	.	.	.	no
C16	C17	C18	C19	-178.5(4)	.	.	.	.	no
C112	C17	C18	C19	1.7(6)	.	.	.	.	no
C16	C17	C112	C113	-3.9(5)	.	.	.	.	no
C17	C18	C19	C110	-1.4(7)	.	.	.	.	no
C18	C19	C110	C111	0.4(6)	.	.	.	.	no
H110	C110	C111	C112	-179.63	.	.	.	.	no
C19	C110	C111	H111	-179.61	.	.	.	.	no
H110	C110	C111	H111	0.35	.	.	.	.	no
H111	C111	C112	C113	3.36	.	.	.	.	no
H111	C111	C112	C17	179.88	.	.	.	.	no
C113	C114	C115	H115	-2.71	.	.	.	.	no
C15	C114	C115	H115	178.61	.	.	.	.	no
C113	C116	C128	H128	-2.17	.	.	.	.	no
C117	C116	C128	H128	178.01	.	.	.	.	no
C117	C118	C119	H119	4.17	.	.	.	.	no
C123	C118	C119	H119	-175.44	.	.	.	.	no
C118	C119	C120	H120	179.45	.	.	.	.	no
H119	C119	C120	H120	-0.54	.	.	.	.	no
H119	C119	C120	C121	179.50	.	.	.	.	no
H120	C120	C121	H121	-2.97	.	.	.	.	no
H120	C120	C121	C122	177.11	.	.	.	.	no
C119	C120	C121	H121	177.00	.	.	.	.	no
C120	C121	C122	H122	-177.83	.	.	.	.	no
H121	C121	C122	C123	-177.79	.	.	.	.	no
H121	C121	C122	H122	2.25	.	.	.	.	no
O21	C22	C23	C24	-177.2(3)	.	.	.	.	no
C23	C22	C215	C214	-0.8(5)	.	.	.	.	no
H122	C122	C123	C124	3.18	.	.	.	.	no
O21	C22	C215	C214	179.8(3)	.	.	.	.	no
H122	C122	C123	C118	-177.99	.	.	.	.	no
C215	C22	C23	C24	3.4(5)	.	.	.	.	no
C122	C123	C124	H124	-3.40	.	.	.	.	no
C22	C23	C24	C25	-1.1(5)	.	.	.	.	no
C118	C123	C124	H124	177.76	.	.	.	.	no
C123	C124	C125	H125	-173.17	.	.	.	.	no
C23	C24	C25	C214	-3.9(5)	.	.	.	.	no
H124	C124	C125	C126	-173.21	.	.	.	.	no
C23	C24	C25	C26	171.2(3)	.	.	.	.	no
H124	C124	C125	H125	6.78	.	.	.	.	no
C214	C25	C26	O22	-162.4(3)	.	.	.	.	no
C214	C25	C26	C27	21.6(4)	.	.	.	.	no
C24	C25	C26	O22	22.5(5)	.	.	.	.	no
H125	C125	C126	C117	177.17	.	.	.	.	no
C24	C25	C26	C27	-153.5(3)	.	.	.	.	no
C26	C25	C214	C215	-168.7(3)	.	.	.	.	no
C24	C25	C214	C215	6.4(4)	.	.	.	.	no
C26	C25	C214	C213	13.0(4)	.	.	.	.	no
H125	C125	C126	N11	-0.38	.	.	.	.	no
C24	C25	C214	C213	-171.9(3)	.	.	.	.	no
O22	C26	C27	C212	156.4(3)	.	.	.	.	no
C25	C26	C27	C212	-27.6(4)	.	.	.	.	no
O22	C26	C27	C28	-24.6(5)	.	.	.	.	no
C25	C26	C27	C28	151.4(3)	.	.	.	.	no

C28	C27	C212	C211	-0.5(4)	.	.	.	.	no
H127	C127	C128	C129	34.25	.	.	.	.	no
H127	C127	C128	H128	-85.54	.	.	.	.	no
C26	C27	C28	C29	-178.0(3)	.	.	.	.	no
N11	C127	C128	H128	153.21	.	.	.	.	no
C28	C27	C212	C213	179.4(3)	.	.	.	.	no
H127	C127	C128	C116	157.75	.	.	.	.	no
C26	C27	C212	C213	-1.6(4)	.	.	.	.	no
H127'	C127	C128	C116	-84.80	.	.	.	.	no
H127'	C127	C128	C129	151.70	.	.	.	.	no
C212	C27	C28	C29	1.0(5)	.	.	.	.	no
H127'	C127	C128	H128	31.91	.	.	.	.	no
C26	C27	C212	C211	178.5(3)	.	.	.	.	no
C27	C28	C29	C210	-0.7(5)	.	.	.	.	no
C116	C128	C129	H129	-66.19	.	.	.	.	no
C127	C128	C129	H129'	-64.96	.	.	.	.	no
C116	C128	C129	H129"	53.82	.	.	.	.	no
C127	C128	C129	H129	55.10	.	.	.	.	no
C116	C128	C129	H129'	173.75	.	.	.	.	no
H128	C128	C129	H129'	54.83	.	.	.	.	no
H128	C128	C129	H129"	-65.10	.	.	.	.	no
C127	C128	C129	H129"	175.11	.	.	.	.	no
H128	C128	C129	H129	174.88	.	.	.	.	no
C28	C29	C210	C211	-0.2(5)	.	.	.	.	no
C134	C131	C132	H132'	-73.74	.	.	.	.	no
C132	C131	C134	H134'	60.49	.	.	.	.	no
C132	C131	C134	H134"	-59.57	.	.	.	.	no
C134	C131	C132	H132"	166.31	.	.	.	.	no
O14	C131	C133	H133"	65.05	.	.	.	.	no
O14	C131	C133	H133	-54.99	.	.	.	.	no
C133	C131	C132	H132	173.74	.	.	.	.	no
C132	C131	C133	H133'	-64.14	.	.	.	.	no
C132	C131	C133	H133"	175.88	.	.	.	.	no
C132	C131	C133	H133	55.84	.	.	.	.	no
C134	C131	C132	H132	46.26	.	.	.	.	no
O14	C131	C133	H133'	-174.96	.	.	.	.	no
C133	C131	C134	H134"	174.02	.	.	.	.	no
C133	C131	C134	H134	54.04	.	.	.	.	no
O14	C131	C132	H132	-70.91	.	.	.	.	no
C133	C131	C132	H132'	53.74	.	.	.	.	no
C133	C131	C132	H132"	-66.21	.	.	.	.	no
O14	C131	C134	H134	-68.16	.	.	.	.	no
C134	C131	C133	H133'	61.78	.	.	.	.	no
C134	C131	C133	H133"	-58.20	.	.	.	.	no
C132	C131	C134	H134	-179.55	.	.	.	.	no
C133	C131	C134	H134'	-65.92	.	.	.	.	no
C134	C131	C133	H133	-178.24	.	.	.	.	no
O14	C131	C134	H134'	171.89	.	.	.	.	no
O14	C131	C134	H134"	51.82	.	.	.	.	no
O14	C131	C132	H132"	49.14	.	.	.	.	no
O14	C131	C132	H132'	169.09	.	.	.	.	no
C29	C210	C211	C212	0.7(5)	.	.	.	.	no
C210	C211	C212	C27	-0.4(4)	.	.	.	.	no
C210	C211	C212	C213	179.8(3)	.	.	.	.	no
C211	C212	C213	C216	45.6(5)	.	.	.	.	no
C27	C212	C213	C214	35.5(4)	.	.	.	.	no
C27	C212	C213	C216	-134.3(3)	.	.	.	.	no
C211	C212	C213	C214	-144.6(3)	.	.	.	.	no
C212	C213	C214	C215	140.4(3)	.	.	.	.	no
C216	C213	C214	C215	-50.0(5)	.	.	.	.	no
C212	C213	C214	C25	-41.4(4)	.	.	.	.	no
C216	C213	C214	C25	128.2(3)	.	.	.	.	no
C212	C213	C216	C228	-178.2(3)	.	.	.	.	no
C214	C213	C216	C217	-170.0(3)	.	.	.	.	no
C212	C213	C216	C217	-1.3(5)	.	.	.	.	no
C214	C213	C216	C228	13.1(5)	.	.	.	.	no

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 C25     C214    C215    C22        -4.1(5)     .       .       .       .   no
 C213    C214    C215    C22       174.0(3)     .       .       .       .   no
 C228    C216    C217    C218     -122.4(3)     .       .       .       .   no
 C213    C216    C217    C218       60.3(5)     .       .       .       .   no
 C213    C216    C217    C226     -131.5(3)     .       .       .       .   no
 C228    C216    C217    C226       45.8(4)     .       .       .       .   no
 C213    C216    C228    C227      108.3(4)     .       .       .       .   no
 C213    C216    C228    C229     -126.9(3)     .       .       .       .   no
 C217    C216    C228    C227      -69.1(3)     .       .       .       .   no
 C217    C216    C228    C229       55.7(4)     .       .       .       .   no
 C216    C217    C218    C223      175.3(3)     .       .       .       .   no
 C226    C217    C218    C219     -171.6(3)     .       .       .       .   no
 C226    C217    C218    C223        7.4(4)     .       .       .       .   no
 C216    C217    C226    N21         3.3(4)     .       .       .       .   no
 C216    C217    C226    C225     -173.0(3)     .       .       .       .   no
 C218    C217    C226    N21       172.0(3)     .       .       .       .   no
 C218    C217    C226    C225       -4.3(4)     .       .       .       .   no
 C216    C217    C218    C219       -3.7(5)     .       .       .       .   no
 C217    C218    C219    C220     -177.5(3)     .       .       .       .   no
 C223    C218    C219    C220        3.4(5)     .       .       .       .   no
 C217    C218    C223    C222      176.5(3)     .       .       .       .   no
 C217    C218    C223    C224       -5.6(4)     .       .       .       .   no
 C219    C218    C223    C222       -4.5(4)     .       .       .       .   no
 C219    C218    C223    C224      173.6(3)     .       .       .       .   no
 C218    C219    C220    C221        0.4(5)     .       .       .       .   no
 C219    C220    C221    C222       -3.3(5)     .       .       .       .   no
 C220    C221    C222    C223        2.2(5)     .       .       .       .   no
 C221    C222    C223    C218        1.8(5)     .       .       .       .   no
 C221    C222    C223    C224     -176.1(3)     .       .       .       .   no
 C222    C223    C224    C225      178.5(3)     .       .       .       .   no
 C218    C223    C224    C225        0.6(5)     .       .       .       .   no
 C223    C224    C225    C226        2.6(5)     .       .       .       .   no
 C224    C225    C226    C217       -0.7(5)     .       .       .       .   no
 C224    C225    C226    N21      -176.9(3)     .       .       .       .   no
 N21     C227    C228    C216       44.9(3)     .       .       .       .   no
 N21     C227    C228    C229      -80.0(3)     .       .       .       .   no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 O12     O22         3.154(4)                    .     2_545               no
 O13     C134        3.009(4)                    .       .                 no
 O13     C133        3.039(6)                    .       .                 no
 O14     C125        2.773(4)                    .       .                 no
 O22     O12         3.154(4)                    .     2_555               no
 O22     C14         3.349(4)                    .     2_555               no
 O23     C232        3.057(4)                    .       .                 no
 O23     C128        3.357(4)                    .     4_654               no
 O23     C233        2.958(4)                    .       .                 no
 O24     C225        2.763(4)                    .       .                 no
 O11     H24           2.8804                    .     4_555               no
 O12     H222          2.8285                    .     1_455               no
 O12     H18           2.6415                    .       .                 no
 O12     H14           2.6470                    .       .                 no
 O12     H28           2.5475                    .     2_545               no
 O13     H228          2.7581                    .     4_555               no
 O13     H229'         2.9027                    .     4_555               no
 O13     H127'         2.5275                    .       .                 no
 O13     H134          2.4496                    .       .                 no
 O13     H127          2.6606                    .       .                 no
 O13     H133"         2.4620                    .       .                 no
 O14     H125          2.3943                    .       .                 no
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O21	H134"	2.7007	.	4_554	no
O22	H122	2.5160	.	.	no
O22	H14	2.8004	.	2_555	no
O22	H24	2.6227	.	.	no
O22	H28	2.6468	.	.	no
O23	H128	2.6073	.	4_654	no
O23	H227	2.5678	.	.	no
O23	H227'	2.5531	.	.	no
O23	H232	2.4884	.	.	no
O23	H233"	2.4324	.	.	no
O24	H225	2.3172	.	.	no
N21	H229	2.9329	.	.	no
C14	O22	3.349(4)	.	2_545	no
C17	C119	3.428(4)	.	.	no
C21	C29	3.594(6)	.	3_665	no
C21	C28	3.492(6)	.	3_665	no
C27	C219	3.528(4)	.	.	no
C28	C21	3.492(6)	.	3_665	no
C29	C21	3.594(6)	.	3_665	no
C111	C118	3.147(4)	.	.	no
C11	H13	2.5862	.	.	no
C111	C119	3.335(5)	.	.	no
C111	C117	3.052(4)	.	.	no
C112	C119	3.050(4)	.	.	no
C112	C118	3.229(4)	.	.	no
C13	H24	2.9716	.	2_545	no
C13	H11	2.7776	.	.	no
C113	C119	3.280(4)	.	.	no
C13	H11"	2.8189	.	.	no
C14	H24	3.0220	.	2_545	no
C115	C128	3.171(4)	.	.	no
C117	C111	3.052(4)	.	.	no
C17	H119	2.8987	.	.	no
C118	C111	3.147(4)	.	.	no
C18	H224	3.0726	.	1_455	no
C118	C112	3.229(4)	.	.	no
C119	C112	3.050(4)	.	.	no
C119	C113	3.280(4)	.	.	no
C119	C17	3.428(4)	.	.	no
C119	C111	3.335(5)	.	.	no
C21	H23	2.5668	.	.	no
C21	H111	2.9535	.	4_554	no
C23	H21	2.7759	.	.	no
C23	H21"	2.8081	.	.	no
C23	H115	3.0763	.	4_554	no
C125	O14	2.773(4)	.	.	no
C126	C129	3.302(5)	.	.	no
C27	H219	2.9153	.	.	no
C128	O23	3.357(4)	.	4_455	no
C128	C115	3.171(4)	.	.	no
C28	H21"	2.8868	.	3_665	no
C28	H124	2.7181	.	.	no
C129	C126	3.302(5)	.	.	no
C29	H21"	2.9364	.	3_665	no
C29	H132"	2.9840	.	.	no
C133	O13	3.039(6)	.	.	no
C134	O13	3.009(4)	.	.	no
C110	H210	3.0926	.	2_645	no
C211	C219	3.462(5)	.	.	no
C211	C218	3.306(4)	.	.	no
C211	C217	3.102(4)	.	.	no
C212	C218	3.323(4)	.	.	no
C212	C219	3.122(4)	.	.	no
C112	H119	2.6876	.	.	no
C113	H119	2.7545	.	.	no
C213	C219	3.309(4)	.	.	no

C114	H128	2.6295	.	.	no
C115	H128	2.4233	.	.	no
C215	C228	3.154(4)	.	.	no
C116	H115	3.0345	.	.	no
C116	H111	2.9620	.	.	no
C116	H119	2.7421	.	.	no
C217	C211	3.102(4)	.	.	no
C117	H129	2.6383	.	.	no
C117	H111	2.6749	.	.	no
C218	C211	3.306(4)	.	.	no
C118	H111	3.0192	.	.	no
C218	C212	3.323(4)	.	.	no
C119	H132'	3.0686	.	1_455	no
C219	C213	3.309(4)	.	.	no
C219	C211	3.462(5)	.	.	no
C219	C212	3.122(4)	.	.	no
C219	C27	3.528(4)	.	.	no
C122	H234	3.0722	.	1_455	no
C123	H18	2.9744	.	2_555	no
C124	H18	2.8649	.	2_555	no
C225	O24	2.763(4)	.	.	no
C226	C229	3.202(5)	.	.	no
C126	H129	2.8048	.	.	no
C228	C215	3.154(4)	.	.	no
C128	H115	2.8190	.	.	no
C229	C226	3.202(5)	.	.	no
C129	H225	3.0703	.	2_655	no
C130	H125	2.8433	.	.	no
C130	H134	2.8724	.	.	no
C130	H133"	2.7074	.	.	no
C232	O23	3.057(4)	.	.	no
C233	O23	2.958(4)	.	.	no
C211	H11	3.0659	.	4_654	no
C212	H219	2.6655	.	.	no
C213	H219	2.7369	.	.	no
C214	H228	2.6397	.	.	no
C215	H228	2.4019	.	.	no
C216	H215	3.0597	.	.	no
C216	H219	2.7222	.	.	no
C216	H211	2.9526	.	.	no
C217	H229	2.6450	.	.	no
C217	H211	2.7146	.	.	no
C223	H120	3.0417	.	1_655	no
C226	H229	2.6833	.	.	no
C227	H134	2.9919	.	4_554	no
C228	H215	2.8110	.	.	no
C229	H229'	2.9487	.	3_655	no
C230	H233"	2.8099	.	.	no
C230	H225	2.8584	.	.	no
C230	H233	3.0282	.	.	no
C230	H232	2.8299	.	.	no
H127'	O13	2.5275	.	.	no
H129'	H225	2.5761	.	2_655	no
H129'	H127	2.4979	.	.	no
H129"	H134'	2.4489	.	1_455	no
H132'	H133'	2.5252	.	.	no
H132'	C119	3.0686	.	1_655	no
H132"	C29	2.9840	.	.	no
H132"	H133	2.5581	.	.	no
H133'	H132'	2.5252	.	.	no
H133"	H134	2.5186	.	.	no
H133"	O13	2.4620	.	.	no
H133"	C130	2.7074	.	.	no
H134'	H129"	2.4489	.	1_655	no
H134"	O21	2.7007	.	4_555	no
H134"	H132	2.4146	.	.	no

H227'	O23	2.5531	.	.	no
H11	C13	2.7776	.	.	no
H11	H13	2.3031	.	.	no
H11	C211	3.0659	.	4_455	no
H11	H211	2.5538	.	4_455	no
H11"	H13	2.4724	.	.	no
H11"	C13	2.8189	.	.	no
H229'	C229	2.9487	.	3_655	no
H229'	H227	2.5414	.	.	no
H229'	H229'	2.4412	.	3_655	no
H229'	O13	2.9027	.	4_554	no
H13	C11	2.5862	.	.	no
H13	H11	2.3031	.	.	no
H13	H11"	2.4724	.	.	no
H232'	H234'	2.5601	.	.	no
H14	O12	2.6470	.	.	no
H14	O22	2.8004	.	2_545	no
H232"	H234	2.5004	.	.	no
H233'	H234'	2.4994	.	.	no
H233"	O23	2.4324	.	.	no
H233"	C230	2.8099	.	.	no
H233"	H232	2.4436	.	.	no
H234'	H233'	2.4994	.	.	no
H234'	H232'	2.5601	.	.	no
H18	O12	2.6415	.	.	no
H18	C123	2.9744	.	2_545	no
H18	C124	2.8649	.	2_545	no
H234"	H233	2.5157	.	.	no
H21	H111	2.5453	.	4_554	no
H21	H23	2.3834	.	.	no
H21	C23	2.7759	.	.	no
H21'	H221	2.5615	.	4_554	no
H21"	C29	2.9364	.	3_665	no
H21"	C23	2.8081	.	.	no
H21"	C28	2.8868	.	3_665	no
H21"	H23	2.3524	.	.	no
H23	H21	2.3834	.	.	no
H23	C21	2.5668	.	.	no
H23	H21"	2.3524	.	.	no
H24	O22	2.6227	.	.	no
H24	C13	2.9716	.	2_555	no
H24	O11	2.8803	.	4_554	no
H24	C14	3.0220	.	2_555	no
H28	O22	2.6468	.	.	no
H28	H124	2.3260	.	.	no
H28	O12	2.5475	.	2_555	no
H111	C117	2.6749	.	.	no
H111	C118	3.0192	.	.	no
H111	C116	2.9620	.	.	no
H111	C21	2.9535	.	4_555	no
H111	H21	2.5453	.	4_555	no
H115	C116	3.0345	.	.	no
H115	C23	3.0763	.	4_555	no
H115	C128	2.8190	.	.	no
H115	H128	2.1220	.	.	no
H119	C116	2.7421	.	.	no
H119	C17	2.8987	.	.	no
H119	C113	2.7545	.	.	no
H119	C112	2.6876	.	.	no
H120	C223	3.0417	.	1_455	no
H121	H211	2.5451	.	1_455	no
H122	O22	2.5160	.	.	no
H122	H124	2.4801	.	.	no
H124	C28	2.7181	.	.	no
H124	H28	2.3260	.	.	no
H124	H122	2.4801	.	.	no

H125	O14	2.3943	.	.	no
H125	C130	2.8433	.	.	no
H127	H129'	2.4979	.	.	no
H127	O13	2.6606	.	.	no
H128	C114	2.6295	.	.	no
H128	O23	2.6073	.	4_455	no
H128	C115	2.4233	.	.	no
H128	H115	2.1220	.	.	no
H129	C126	2.8048	.	.	no
H129	C117	2.6383	.	.	no
H132	H134"	2.4146	.	.	no
H133	H132"	2.5581	.	.	no
H134	O13	2.4496	.	.	no
H134	C130	2.8724	.	.	no
H134	H133"	2.5186	.	.	no
H134	C227	2.9919	.	4_555	no
H210	C110	3.0926	.	2_655	no
H211	C216	2.9526	.	.	no
H211	C217	2.7146	.	.	no
H211	H121	2.5451	.	1_655	no
H211	H11	2.5538	.	4_654	no
H215	C216	3.0597	.	.	no
H215	C228	2.8110	.	.	no
H215	H228	2.1119	.	.	no
H219	C27	2.9153	.	.	no
H219	C212	2.6655	.	.	no
H219	C213	2.7369	.	.	no
H219	C216	2.7222	.	.	no
H221	H21'	2.5615	.	4_555	no
H222	O12	2.8285	.	1_655	no
H222	H224	2.4901	.	.	no
H224	C18	3.0726	.	1_655	no
H224	H222	2.4901	.	.	no
H225	O24	2.3172	.	.	no
H225	C230	2.8584	.	.	no
H225	C129	3.0703	.	2_645	no
H225	H129'	2.5761	.	2_645	no
H227	O23	2.5678	.	.	no
H227	H229'	2.5414	.	.	no
H228	C214	2.6397	.	.	no
H228	C215	2.4019	.	.	no
H228	H215	2.1119	.	.	no
H228	O13	2.7581	.	4_554	no
H229	N21	2.9329	.	.	no
H229	C217	2.6450	.	.	no
H229	C226	2.6833	.	.	no
H232	O23	2.4884	.	.	no
H232	C230	2.8299	.	.	no
H232	H233"	2.4436	.	.	no
H233	C230	3.0282	.	.	no
H233	H234"	2.5157	.	.	no
H234	C122	3.0722	.	1_655	no
H234	H232"	2.5004	.	.	no

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loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
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#
C133    H133"   O13         0.9600     2.4600   3.039(6)     118.00     .   yes
C233    H233"   O23         0.9600     2.4300   2.958(4)     114.00     .   yes
C28     H28     O12         0.9300     2.5500   3.421(5)     157.00   2_555 yes
C122    H122    O22         0.9300     2.5200   3.423(4)     165.00     .   yes
C125    H125    O14         0.9300     2.3900   2.773(4)     104.00     .   yes
C134    H134    O13         0.9600     2.4500   3.009(4)     117.00     .   yes
C225    H225    O24         0.9300     2.3200   2.763(4)     109.00     .   yes
C232    H232    O23         0.9600     2.4900   3.057(4)     118.00     .   yes

#===END of Crystallographic Information File
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