University of Groningen

Influence of the solvent on the crystal structure of PCBM and the efficiency of MDMO-PPV

Rispens, MT; Meetsma, A; Rittberger, R; Brabec, CJ; Sariciftci, NS; Hummelen, JC

Published in:
Chemical Communications

DOI:
[10.1039/b305988j](https://doi.org/10.1039/b305988j)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2003

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Rispens, MT., Meetsma, A., Rittberger, R., Brabec, C.J., Sariciftci, NS., & Hummelen, J.C. (2003). Influence of the solvent on the crystal structure of PCBM and the efficiency of MDMO-PPV: PCBM 'plastic' solar cells. *Chemical Communications*, (17), 2116-2118. <https://doi.org/10.1039/b305988j>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

```
data_global
_journal_name_full          Chem.Commun.
#=====

# 0. AUDIT DETAILS

_audit_creation_date        '2001-03-06  15:24:09'
_audit_creation_method
;
PLATON <TABLE ACC> option
SHELXL97-2 & Manual Editing
;
_audit_update_record
;
2003_06-30

Impact of setting C44 to isotropic displacement parameter

;

_journal_codен_Cambridge    0182

_publ_contact_author_name   'Prof Jan C. Hummelen'
_publ_contact_author_address
;
Molecular Electronics, MSC
Groningen University
Nijenborgh 4
Groningen
9747 AG
NETHERLANDS
;

_publ_contact_author_email   J.C.HUMMELEN@CHEM.RUG.NL

_publ_contact_letter        # Include date of submission
;

Date of submission :  2003-05-25

Consider this CIF submission for deposition of the second
X-ray structure of the manuscript entitled:

Influence of the solvent on the crystal structure of PCBM and the
efficiency of MDMO-PPV:PCBM 'plastic' solar cells
(Our Compound_Identification_Code: CP578B)
;

_publ_section_title
;
Influence of the solvent on the crystal structure of PCBM and the
efficiency of MDMO-PPV:PCBM 'plastic' solar cells
;

loop_
_publ_author_name
_publ_author_address

M.T.Rispens
;
Molecular Electronics, MSC+,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen,
```

The Netherlands.

;

A.Meetsma

;

Molecular Electronics, MSC+,
Groningen University,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.

;

R.Rittberger

;

Linz Institute for Organic Solar Cells (LIOS),
Physical Chemistry,
Johannes Kepler University of Linz,
Altenbergerstr. 69
A-4040 Linz,
Austria.

;

C.J.Brabec

;

Siemens AG,
CT MM1,
Innovative Electronics,
Paul-Gossen-Str 100,
D-91052 Erlangen,
Germany.

;

N.S.Sariciftci

;

Linz Institute for Organic Solar Cells (LIOS),
Physical Chemistry,
Johannes Kepler University of Linz,
Altenbergerstr. 69
A-4040 Linz,
Austria.

;

;

J.C.Hummelen

;

;

Molecular Electronics, MSC+,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.

;

#####

_publ_section_exptl_refinement

;

Refinement was complicated (frustrated) by a disorder problem: from the solution it was clear that the chlorobenzene solvent molecules were (highly) disordered over an inversion centre (residue 3 on (0.0,.0.5,0.0) and residue 4 on (0.0,0.5,0.5)).

The electron density of the chloride and the carbon atoms appeared to be spread out, indicating translation disorder. A disorder model (50:50) with bond restraints ("variable metric rigid hexagon") was used in the refinement. The C44 position converged to non-positive definite displacement parameters when allowed to vary anisotropically, so ultimately this was returned to an isotropic displacement parameter.

A subsequent difference Fourier synthesis resulted in the location of all the hydrogen atoms which co-ordinates and isotropic displacement parameters were refined, except those belonging to disordered C atoms of the chlorobenzene solvent molecules, which were constrained to idealised

geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms.

;

Insert blank lines between references

_publ_section_references

;

Altomare, A., Burla, M.C., Camalli, M., Cascarano, G.L., Giacovazzo, C. Guagliardi, A., Moliterni, A.G.G., Polidori, G. & Spagna, R. (1999). J. Appl. Cryst. 32, 115-119.

Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

Bruker, (2000). SMART, SAINT, SADABS, XPREP and SHELXTL/NT. Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

International Tables for Crystallography (1983). Vol. A. Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht).

International Tables for Crystallography (1992). Vol. C. Edited by A.J.C Wilson, Kluwer Academic Publishers, Dordrecht, The Netherlands.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2000). Extended version of the program PLUTO. Groningen University, The Netherlands. (unpublished).

Sheldrick, G.M. SHELXL97. Program for Crystal Structure Refinement. University of Gottingen, Germany, 1997.

Sheldrick, G.M. SADABS. Version 2. Multi-Scan Absorption Correction Program. University of Gottingen, Germany, 2001

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

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

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 are drawn with an arbitrary radius.

;

#####

data_c78h18cl

_database_code_CSD

211976

```

_audit_creation_date      '2001-01-03 16:10:48'
_audit_creation_method    'PLATON <TABLE ACC> option'
_audit_update_record
;
?
;

#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
;
Methyl 5-(3'H-cyclopropa[1,9](C60-Ih)[5,6]fullerenyl)-5-phenylpentanoate.
;
_chemical_name_common      'Phenyl-C61-Butyric acid Methyl ester (PCBM)'
_chemical_melting_point    ?
_chemical_formula_moiety    'C72 H14 O2, C6 H4 Cl2'
_chemical_formula_structural ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum        'C78 H18 Cl2 O2'
_chemical_formula_weight     1057.91
_chemical_compound_source    'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

# 6. CRYSTAL DATA

_symmetry_cell_setting      Monoclinic
_symmetry_space_group_name_Hall '-P 2yn'
_symmetry_space_group_name_H-M 'P 21/n'

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
1/2-x,1/2+y,1/2-z
-x,-y,-z
1/2+x,1/2-y,1/2+z

_cell_length_a              13.7565(9)
_cell_length_b              16.634(1)
_cell_length_c              19.077(1)
_cell_angle_alpha           90
_cell_angle_beta            105.289(1)
_cell_angle_gamma           90
_cell_volume                4210.8(4)
_cell_formula_units_Z       4
_cell_measurement_temperature 90
_cell_measurement_reflns_used 3065
_cell_measurement_theta_min  2.44
_cell_measurement_theta_max  25.20
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
3065 reflections after integration using the SAINT software
package (Bruker, 2000).

```

The intensity data were corrected for decay and absorption using SADABS (Sheldrick, 2000).

```
;
_exptl_crystal_description      '  platelet'
_exptl_crystal_colour          '  red-brown'
_exptl_crystal_size_max        0.250
_exptl_crystal_size_mid        0.200
_exptl_crystal_size_min        0.020
_exptl_crystal_size_rad        ?
_exptl_crystal_density_meas    ?
_exptl_crystal_density_diffn   1.669
_exptl_crystal_density_method  'Not Measured'
_exptl_crystal_F_000           2144
_exptl_absorpt_coefficient_mu   0.221
_exptl_absorpt_correction_type  Semi-empirical
_exptl_absorpt_process_details '(SADABS (Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.9280
_exptl_absorpt_correction_T_max 1.0000
```

#=====

7. EXPERIMENTAL DATA

```
_exptl_special_details
;
?
;

_diffn_ambient_temperature      90(r12)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK\alpha
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;
_diffn_measurement_device_type
;
Bruker Smart Apex
;

_diffn_measurement_method       'phi and omega scans'

_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature
unit (KROFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean ?

_diffn_standards_number         ?
_diffn_standards_interval_count ?
_diffn_standards_interval_time  ?
_diffn_standards_decay_%        negligible

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number            25918
_diffn_reflns_av_R_equivalents  0.0630
_diffn_reflns_av_sigmaI/netI    0.1710
```

```

_diffrn_reflms_limit_h_min      -16
_diffrn_reflms_limit_h_max      17
_diffrn_reflms_limit_k_min      -21
_diffrn_reflms_limit_k_max      15
_diffrn_reflms_limit_l_min      -24
_diffrn_reflms_limit_l_max      22
_diffrn_reflms_theta_min        2.44
_diffrn_reflms_theta_max        27.53
_diffrn_measured_fraction_theta_max 0.962
_diffrn_reflms_theta_full       27.53
_diffrn_measured_fraction_theta_full 0.962

```

```
_diffrn_reflms_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 SABABS (Sheldrick, 2000)
;

```

```
# number of unique reflections
```

```

_reflms_number_total      9661
_reflms_number_gt         4425
_reflms_threshold_expression >2sigma(I)

```

```

_computing_data_collection 'SMART, Bruker Version 5.168, 2000'
_computing_cell_refinement 'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction  'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;

```

```
SIR-97 (Altomare et al., 1997)
```

```

;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;

```

```
PLUTO (Meetsma, 2000)
```

```
PLATON (Spek, 1994, 1996)
```

```

;
_computing_publication_material
;

```

```
PLATON (Spek, 1990)
```

```
SHELXL (Sheldrick, 1997)
```

```
;
```

```
#####
```

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 $F^2 > 2\sigma(F^2)$ 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_details calc
```

```
_refine_ls_weighting_scheme
```

```
'calc w=1/[\s^2*(Fo^2)+(0.0147P)^2+0.0000P] where P=(Fo^2+2Fc^2)/3'
```

```
_atom_sites_solution_primary Patterson
```

```
_atom_sites_solution_secondary direct
```

```
_atom_sites_solution_hydrogens difmap
```

```
_refine_ls_hydrogen_treatment refall
```

<u>refine_ls_extinction_method</u>	none
<u>refine_ls_extinction_coef</u>	?
<u>refine_ls_abs_structure_details</u>	?
<u>refine_ls_abs_structure_Flack</u>	?
<u>refine_ls_number_reflns</u>	9661
<u>refine_ls_number_parameters</u>	811
<u>refine_ls_number_restraints</u>	0
<u>refine_ls_number_constraints</u>	?
<u>refine_ls_R_factor_all</u>	0.1084
<u>refine_ls_R_factor_gt</u>	0.0442
<u>refine_ls_wR_factor_ref</u>	0.0701
<u>refine_ls_wR_factor_gt</u>	0.0621
<u>refine_ls_goodness_of_fit_ref</u>	0.687
<u>refine_ls_restrained_S_all</u>	0.687
<u>refine_ls_shift/su_max</u>	0.000
<u>refine_ls_shift/su_mean</u>	0.000
<u>refine_diff_density_max</u>	0.375
<u>refine_diff_density_min</u>	-0.395
<u>refine_diff_density_rms</u>	0.054

9. ATOMIC COORDINATES AND THERMAL PARAMETERS

C01	O	Uani	0.30167(12)	0.25012(11)	0.16769(9)	1.000	0.0307(7)
C02	O	Uani	0.46681(12)	0.27914(10)	0.19456(8)	1.000	0.0218(6)
C01	C	Uani	0.21552(17)	0.18439(15)	0.39206(12)	1.000	0.0156(8)
C02	C	Uani	0.16516(17)	0.12651(15)	0.32347(12)	1.000	0.0147(8)
C03	C	Uani	0.08339(17)	0.07276(14)	0.33397(13)	1.000	0.0152(8)
C04	C	Uani	0.05938(17)	0.06441(14)	0.39948(13)	1.000	0.0167(8)
C05	C	Uani	0.10516(18)	0.11667(16)	0.46158(13)	1.000	0.0193(9)
C06	C	Uani	0.17293(17)	0.17526(16)	0.45591(12)	1.000	0.0167(9)
C07	C	Uani	0.16444(17)	0.25449(16)	0.48457(12)	1.000	0.0177(8)
C08	C	Uani	0.18729(17)	0.31365(16)	0.43548(13)	1.000	0.0183(9)
C09	C	Uani	0.20972(16)	0.27147(15)	0.37531(13)	1.000	0.0160(8)
C10	C	Uani	0.17644(17)	0.30312(15)	0.30666(13)	1.000	0.0166(9)
C11	C	Uani	0.12966(17)	0.25066(15)	0.24431(12)	1.000	0.0162(8)
C12	C	Uani	0.12026(17)	0.16925(15)	0.25396(12)	1.000	0.0149(8)
C13	C	Uani	0.02684(17)	0.12996(16)	0.21822(12)	1.000	0.0177(9)
C14	C	Uani	0.00401(17)	0.07132(15)	0.26755(13)	1.000	0.0169(8)
C15	C	Uani	-0.09529(18)	0.05664(15)	0.26691(13)	1.000	0.0189(9)
C16	C	Uani	-0.12048(17)	0.04569(15)	0.33530(13)	1.000	0.0180(9)
C17	C	Uani	-0.04491(18)	0.05061(15)	0.39978(13)	1.000	0.0191(9)
C18	C	Uani	-0.06378(18)	0.09280(16)	0.46164(13)	1.000	0.0208(9)
C19	C	Uani	0.02800(18)	0.13403(16)	0.49922(12)	1.000	0.0194(9)
C20	C	Uani	0.02316(18)	0.20932(17)	0.52948(12)	1.000	0.0203(9)
C21	C	Uani	0.09253(18)	0.27151(17)	0.52204(12)	1.000	0.0197(9)
C22	C	Uani	0.04032(18)	0.34793(16)	0.51164(13)	1.000	0.0219(9)
C23	C	Uani	0.06231(18)	0.40426(16)	0.46451(13)	1.000	0.0218(9)
C24	C	Uani	0.13779(17)	0.38746(16)	0.42581(13)	1.000	0.0204(9)
C25	C	Uani	0.10469(17)	0.42065(15)	0.35414(13)	1.000	0.0194(9)
C26	C	Uani	0.12236(17)	0.37890(15)	0.29525(13)	1.000	0.0191(9)
C27	C	Uani	0.04436(18)	0.37426(16)	0.22755(13)	1.000	0.0207(9)
C28	C	Uani	0.04926(18)	0.29563(16)	0.19668(13)	1.000	0.0190(9)
C29	C	Uani	-0.03941(18)	0.25652(16)	0.15980(12)	1.000	0.0200(9)
C30	C	Uani	-0.05055(18)	0.17218(16)	0.17106(12)	1.000	0.0191(9)
C31	C	Uani	-0.15473(18)	0.15757(16)	0.17117(12)	1.000	0.0188(9)

C32 C Uani -0.17652(17) 0.10075(15) 0.21822(13) 1.000 0.0192(9)
C33 C Uani -0.25188(17) 0.11764(16) 0.25686(13) 1.000 0.0195(9)
C34 C Uani -0.21750(18) 0.08424(15) 0.32918(14) 1.000 0.0218(9)
C35 C Uani -0.23565(18) 0.12445(16) 0.38782(14) 1.000 0.0207(9)
C36 C Uani -0.15693(18) 0.12941(16) 0.45572(13) 1.000 0.0205(9)
C37 C Uani -0.16217(18) 0.20785(16) 0.48687(13) 1.000 0.0210(9)
C38 C Uani -0.07377(18) 0.24756(17) 0.52329(12) 1.000 0.0211(9)
C39 C Uani -0.06328(19) 0.33307(17) 0.51227(12) 1.000 0.0211(10)
C40 C Uani -0.14123(18) 0.37545(16) 0.46556(13) 1.000 0.0214(9)
C41 C Uani -0.11811(18) 0.43470(15) 0.41612(13) 1.000 0.0222(9)
C42 C Uani -0.01842(18) 0.44887(15) 0.41573(13) 1.000 0.0205(9)
C43 C Uani 0.00784(18) 0.45890(15) 0.34729(14) 1.000 0.0221(9)
C44 C Uani -0.06671(19) 0.45434(15) 0.28233(14) 1.000 0.0229(9)
C45 C Uani -0.04817(19) 0.41175(15) 0.22108(13) 1.000 0.0215(9)
C46 C Uani -0.14084(18) 0.37089(16) 0.18289(13) 1.000 0.0208(9)
C47 C Uani -0.13623(18) 0.29583(17) 0.15301(12) 1.000 0.0210(9)
C48 C Uani -0.20703(18) 0.23371(17) 0.16039(12) 1.000 0.0207(9)
C49 C Uani -0.27978(17) 0.25014(17) 0.19717(13) 1.000 0.0202(9)
C50 C Uani -0.30278(17) 0.19098(16) 0.24639(13) 1.000 0.0203(9)
C51 C Uani -0.32178(17) 0.23346(16) 0.30797(13) 1.000 0.0182(9)
C52 C Uani -0.28847(17) 0.20073(16) 0.37709(14) 1.000 0.0201(9)
C53 C Uani -0.24323(18) 0.25247(16) 0.43855(13) 1.000 0.0193(9)
C54 C Uani -0.23251(18) 0.33379(16) 0.42761(13) 1.000 0.0195(9)
C55 C Uani -0.26694(17) 0.36802(16) 0.35510(13) 1.000 0.0193(9)
C56 C Uani -0.31056(17) 0.31869(16) 0.29690(13) 1.000 0.0193(9)
C57 C Uani -0.28481(17) 0.32900(16) 0.22827(13) 1.000 0.0207(9)
C58 C Uani -0.21662(17) 0.38804(16) 0.22102(13) 1.000 0.0205(9)
C59 C Uani -0.17055(18) 0.43967(15) 0.28304(14) 1.000 0.0203(9)
C60 C Uani -0.19594(18) 0.42983(15) 0.34839(13) 1.000 0.0202(9)
C61 C Uani 0.27592(17) 0.12167(15) 0.36385(12) 1.000 0.0178(8)
C62 C Uani 0.31030(17) 0.04927(15) 0.41092(13) 1.000 0.0168(8)
C63 C Uani 0.35860(18) 0.05901(17) 0.48445(14) 1.000 0.0199(9)
C64 C Uani 0.39384(18) -0.00750(17) 0.52827(15) 1.000 0.0226(10)
C65 C Uani 0.38183(18) -0.08382(17) 0.49845(15) 1.000 0.0213(10)
C66 C Uani 0.33468(18) -0.09416(17) 0.42532(15) 1.000 0.0218(9)
C67 C Uani 0.29842(18) -0.02808(16) 0.38184(14) 1.000 0.0196(9)
C68 C Uani 0.35108(19) 0.15337(16) 0.32371(14) 1.000 0.0176(9)
C69 C Uani 0.35346(19) 0.10560(16) 0.25585(14) 1.000 0.0187(9)
C70 C Uani 0.4233(2) 0.14578(16) 0.21527(15) 1.000 0.0209(9)
C71 C Uani 0.38872(19) 0.22948(17) 0.19016(13) 1.000 0.0203(9)
C72 C Uani 0.4415(2) 0.36232(18) 0.17376(17) 1.000 0.0260(10)
C11 Cl Uani 0.41388(5) 0.39302(4) 0.35693(3) 1.000 0.0314(3)
C12 Cl Uani 0.46934(5) 0.26987(4) 0.48695(3) 1.000 0.0316(3)
C73 C Uani 0.51598(17) 0.41028(16) 0.43143(12) 1.000 0.0190(9)
C74 C Uani 0.54048(18) 0.35682(15) 0.48876(13) 1.000 0.0207(9)
C75 C Uani 0.62126(19) 0.37129(18) 0.54799(14) 1.000 0.0243(10)
C76 C Uani 0.67732(19) 0.44094(19) 0.55001(15) 1.000 0.0273(10)
C77 C Uani 0.6522(2) 0.49505(18) 0.49267(15) 1.000 0.0263(10)
C78 C Uani 0.57226(19) 0.47956(17) 0.43304(14) 1.000 0.0221(10)
H63 H Uiso 0.3669(16) 0.1161(15) 0.5047(12) 1.000 0.036(8)
H64 H Uiso 0.4317(15) 0.0015(13) 0.5816(11) 1.000 0.018(7)
H65 H Uiso 0.4108(15) -0.1315(14) 0.5297(11) 1.000 0.026(7)
H66 H Uiso 0.3224(15) -0.1483(14) 0.4023(11) 1.000 0.018(7)
H67 H Uiso 0.2609(15) -0.0417(14) 0.3289(12) 1.000 0.025(7)
H68 H Uiso 0.3322(15) 0.2107(14) 0.3092(11) 1.000 0.025(7)
H68' H Uiso 0.4253(15) 0.1541(13) 0.3617(10) 1.000 0.019(6)
H69 H Uiso 0.2809(16) 0.1024(13) 0.2189(11) 1.000 0.025(7)
H69' H Uiso 0.3771(14) 0.0485(13) 0.2708(10) 1.000 0.015(6)
H70 H Uiso 0.4929(16) 0.1491(14) 0.2466(12) 1.000 0.029(7)
H70' H Uiso 0.4252(16) 0.1156(15) 0.1691(12) 1.000 0.038(8)
H72 H Uiso 0.3920(16) 0.3649(14) 0.1277(12) 1.000 0.026(7)
H72' H Uiso 0.4102(19) 0.3879(18) 0.2143(14) 1.000 0.075(11)
H72'' H Uiso 0.510(2) 0.3863(17) 0.1708(13) 1.000 0.065(10)
H75 H Uiso 0.6375(17) 0.3363(15) 0.5906(12) 1.000 0.039(8)
H76 H Uiso 0.7309(15) 0.4524(13) 0.5937(11) 1.000 0.021(7)
H77 H Uiso 0.6942(15) 0.5499(14) 0.4958(11) 1.000 0.026(7)
H78 H Uiso 0.5514(16) 0.5203(14) 0.3901(12) 1.000 0.033(8)

```

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
O1 0.0221(11) 0.0352(13) 0.0358(11) 0.0142(10) 0.0092(9) 0.0051(9)
O2 0.0226(10) 0.0169(11) 0.0252(10) 0.0018(9) 0.0049(8) -0.0012(9)
C1 0.0152(14) 0.0179(16) 0.0123(13) -0.0015(12) 0.0010(11) 0.0007(12)
C2 0.0170(14) 0.0122(15) 0.0150(13) -0.0017(12) 0.0046(11) 0.0006(11)
C3 0.0163(14) 0.0113(15) 0.0176(14) -0.0005(12) 0.0039(12) 0.0033(11)
C4 0.0173(14) 0.0101(15) 0.0240(15) 0.0044(12) 0.0076(12) 0.0046(11)
C5 0.0202(15) 0.0206(17) 0.0166(14) 0.0076(13) 0.0042(12) 0.0076(12)
C6 0.0149(14) 0.0234(17) 0.0107(13) 0.0005(12) 0.0012(11) 0.0033(12)
C7 0.0114(13) 0.0241(17) 0.0135(13) -0.0038(13) -0.0041(11) 0.0021(12)
C8 0.0114(14) 0.0205(17) 0.0203(15) -0.0043(13) -0.0006(12) -0.0024(12)
C9 0.0088(13) 0.0175(16) 0.0222(14) -0.0037(13) 0.0051(11) -0.0047(11)
C10 0.0118(14) 0.0144(16) 0.0244(15) 0.0005(12) 0.0064(12) -0.0044(11)
C11 0.0165(14) 0.0177(16) 0.0168(14) -0.0002(12) 0.0086(11) -0.0009(12)
C12 0.0176(14) 0.0196(16) 0.0111(13) -0.0002(12) 0.0099(12) 0.0029(12)
C13 0.0195(15) 0.0226(17) 0.0119(13) -0.0049(12) 0.0058(12) 0.0008(12)
C14 0.0174(14) 0.0111(15) 0.0236(15) -0.0064(12) 0.0081(12) 0.0007(11)
C15 0.0214(15) 0.0123(16) 0.0233(15) -0.0091(13) 0.0066(13) -0.0044(12)
C16 0.0169(14) 0.0095(15) 0.0278(16) -0.0018(12) 0.0062(13) -0.0036(11)
C17 0.0210(15) 0.0114(15) 0.0269(16) 0.0069(13) 0.0099(13) 0.0008(12)
C18 0.0257(16) 0.0196(17) 0.0202(15) 0.0081(13) 0.0117(13) 0.0009(13)
C19 0.0209(15) 0.0256(18) 0.0115(14) 0.0088(12) 0.0040(12) 0.0065(13)
C20 0.0218(15) 0.0291(19) 0.0107(14) 0.0032(13) 0.0055(12) 0.0043(13)
C21 0.0184(15) 0.0280(18) 0.0099(13) -0.0044(13) -0.0011(11) 0.0039(13)
C22 0.0231(16) 0.0274(18) 0.0128(14) -0.0114(13) 0.0003(12) -0.0003(13)
C23 0.0205(15) 0.0176(17) 0.0251(15) -0.0140(14) 0.0019(13) -0.0002(13)
C24 0.0156(14) 0.0161(16) 0.0273(16) -0.0080(13) 0.0017(12) -0.0040(12)
C25 0.0169(15) 0.0118(16) 0.0287(16) 0.0005(13) 0.0046(13) -0.0040(12)
C26 0.0177(14) 0.0120(16) 0.0292(16) 0.0052(13) 0.0088(13) -0.0056(12)
C27 0.0236(15) 0.0179(17) 0.0221(15) 0.0104(13) 0.0086(13) -0.0007(13)
C28 0.0200(15) 0.0243(18) 0.0159(14) 0.0038(13) 0.0105(12) -0.0004(13)
C29 0.0252(16) 0.0271(18) 0.0091(13) 0.0036(13) 0.0070(12) 0.0025(13)
C30 0.0218(15) 0.0233(17) 0.0121(14) -0.0037(13) 0.0045(12) 0.0004(13)
C31 0.0180(15) 0.0252(18) 0.0108(13) -0.0091(13) -0.0003(12) -0.0040(13)
C32 0.0162(14) 0.0154(16) 0.0221(15) -0.0130(13) -0.0018(12) -0.0043(12)
C33 0.0132(14) 0.0178(17) 0.0245(15) -0.0050(13) -0.0003(12) -0.0050(12)
C34 0.0172(15) 0.0137(16) 0.0360(17) 0.0010(14) 0.0099(13) -0.0066(12)
C35 0.0176(15) 0.0184(17) 0.0301(16) 0.0046(14) 0.0134(13) -0.0040(12)
C36 0.0189(15) 0.0245(18) 0.0230(15) 0.0090(13) 0.0140(12) 0.0010(13)
C37 0.0220(15) 0.0298(19) 0.0159(14) 0.0017(13) 0.0135(12) 0.0038(13)
C38 0.0220(15) 0.033(2) 0.0094(13) 0.0012(13) 0.0061(12) 0.0052(14)
C39 0.0226(16) 0.0278(19) 0.0138(14) -0.0058(13) 0.0066(12) 0.0020(13)
C40 0.0232(16) 0.0235(18) 0.0184(14) -0.0063(13) 0.0069(13) 0.0056(13)
C41 0.0223(16) 0.0161(17) 0.0296(16) -0.0098(13) 0.0093(13) 0.0041(12)
C42 0.0226(16) 0.0087(15) 0.0294(16) -0.0074(13) 0.0053(13) -0.0022(12)
C43 0.0240(16) 0.0078(15) 0.0344(17) -0.0034(13) 0.0077(14) -0.0022(12)
C44 0.0245(16) 0.0121(16) 0.0337(17) 0.0060(14) 0.0104(14) 0.0021(12)
C45 0.0266(16) 0.0155(16) 0.0231(15) 0.0105(13) 0.0079(13) 0.0025(13)
C46 0.0228(16) 0.0219(18) 0.0169(14) 0.0093(13) 0.0036(12) 0.0032(13)
C47 0.0227(16) 0.0305(19) 0.0077(13) 0.0060(13) 0.0002(12) 0.0032(13)
C48 0.0201(15) 0.0273(18) 0.0103(13) -0.0012(13) -0.0039(11) 0.0036(13)
C49 0.0129(14) 0.0292(19) 0.0156(14) -0.0004(13) -0.0014(11) 0.0000(12)
C50 0.0089(14) 0.0241(18) 0.0244(15) -0.0035(14) -0.0016(12) 0.0027(12)
C51 0.0120(14) 0.0225(17) 0.0204(15) -0.0033(13) 0.0047(12) -0.0004(12)
C52 0.0120(14) 0.0219(17) 0.0293(16) 0.0002(13) 0.0103(12) -0.0032(12)
C53 0.0186(14) 0.0239(18) 0.0196(14) 0.0007(13) 0.0123(12) 0.0037(13)
C54 0.0169(15) 0.0232(18) 0.0220(15) -0.0032(13) 0.0114(12) 0.0069(13)
C55 0.0147(14) 0.0173(16) 0.0251(15) -0.0015(13) 0.0041(12) 0.0053(12)
C56 0.0102(14) 0.0241(17) 0.0224(15) 0.0018(14) 0.0022(12) 0.0043(12)

```

```

C57 0.0113(14) 0.0246(18) 0.0221(15) 0.0049(13) -0.0026(12) 0.0067(12)
C58 0.0159(14) 0.0226(17) 0.0211(15) 0.0086(13) 0.0014(12) 0.0074(13)
C59 0.0201(15) 0.0109(16) 0.0289(16) 0.0042(13) 0.0049(13) 0.0079(12)
C60 0.0203(15) 0.0148(16) 0.0248(15) -0.0010(13) 0.0047(13) 0.0059(12)
C61 0.0198(15) 0.0182(16) 0.0157(13) -0.0028(12) 0.0051(12) -0.0006(12)
C62 0.0107(12) 0.0215(16) 0.0203(14) 0.0017(14) 0.0076(11) 0.0021(12)
C63 0.0156(15) 0.0224(18) 0.0233(16) -0.0036(14) 0.0080(12) -0.0005(13)
C64 0.0162(15) 0.0279(19) 0.0235(16) 0.0028(14) 0.0051(13) 0.0014(13)
C65 0.0189(15) 0.0194(18) 0.0291(17) 0.0089(14) 0.0126(13) 0.0038(13)
C66 0.0184(15) 0.0181(17) 0.0323(17) -0.0003(15) 0.0129(13) 0.0005(13)
C67 0.0159(15) 0.0200(17) 0.0244(16) -0.0014(14) 0.0077(13) -0.0009(12)
C68 0.0161(15) 0.0178(17) 0.0193(15) 0.0021(13) 0.0055(12) 0.0008(12)
C69 0.0207(15) 0.0138(16) 0.0236(15) 0.0009(14) 0.0093(13) 0.0020(13)
C70 0.0227(16) 0.0171(17) 0.0251(16) -0.0013(14) 0.0101(14) 0.0014(13)
C71 0.0226(16) 0.0241(18) 0.0166(14) -0.0039(13) 0.0096(13) 0.0016(13)
C72 0.0312(19) 0.0150(17) 0.0298(18) 0.0032(15) 0.0047(16) 0.0011(14)
C11 0.0312(4) 0.0376(5) 0.0217(4) 0.0003(3) 0.0002(3) -0.0092(4)
C12 0.0448(5) 0.0234(4) 0.0282(4) 0.0002(3) 0.0127(3) -0.0088(4)
C73 0.0161(14) 0.0241(17) 0.0163(14) -0.0069(13) 0.0033(11) 0.0003(12)
C74 0.0222(15) 0.0186(16) 0.0245(15) -0.0041(13) 0.0119(13) -0.0011(13)
C75 0.0241(16) 0.032(2) 0.0181(15) -0.0024(15) 0.0078(13) 0.0047(14)
C76 0.0158(16) 0.041(2) 0.0228(17) -0.0111(16) 0.0008(14) 0.0027(14)
C77 0.0177(16) 0.0274(19) 0.0354(18) -0.0082(15) 0.0100(14) -0.0051(14)
C78 0.0236(16) 0.0216(18) 0.0220(16) 0.0004(14) 0.0077(13) -0.0005(13)

```

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds 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

C11 C73 1.738(2) . . yes

C12 C74 1.742(3) . . yes

O1 C71 1.210(3) . . yes

O2 C71 1.340(3) . . yes

O2 C72 1.456(3) . . yes

C1 C2 1.625(3) . . no

C1 C61 1.518(3) . . no

C1 C6 1.492(3) . . no

C1 C9 1.481(4) . . no

C2 C3 1.491(3) . . no

C2 C12 1.488(3) . . no

C2 C61 1.517(3) . . no

C3 C4 1.381(3) . . no

C3 C14 1.438(3) . . no

C4 C5 1.470(3) . . no

C4 C17 1.454(4) . . no

C5 C19 1.459(4) . . no

C5 C6 1.373(4) . . no

C6 C7 1.443(4) . . no

C7 C21 1.394(3) . . no

C7 C8 1.449(4) . . no

C8 C24 1.392(4) . . no

C8 C9 1.446(3) . . no
C9 C10 1.373(3) . . no
C10 C11 1.479(3) . . no
C10 C26 1.451(4) . . no
C11 C28 1.442(3) . . no
C11 C12 1.377(4) . . no
C12 C13 1.443(3) . . no
C13 C14 1.446(3) . . no
C13 C30 1.390(3) . . no
C14 C15 1.385(4) . . no
C15 C32 1.450(3) . . no
C15 C16 1.447(3) . . no
C16 C17 1.388(3) . . no
C16 C34 1.457(4) . . no
C17 C18 1.454(3) . . no
C18 C36 1.396(4) . . no
C18 C19 1.449(4) . . no
C19 C20 1.388(4) . . no
C20 C21 1.440(4) . . no
C20 C38 1.454(4) . . no
C21 C22 1.448(4) . . no
C22 C23 1.386(4) . . no
C22 C39 1.450(4) . . no
C23 C24 1.451(4) . . no
C23 C42 1.451(4) . . no
C24 C25 1.433(3) . . no
C25 C26 1.396(3) . . no
C25 C43 1.451(4) . . no
C26 C27 1.447(3) . . no
C27 C28 1.443(4) . . no
C27 C45 1.393(4) . . no
C28 C29 1.398(4) . . no
C29 C47 1.459(4) . . no
C29 C30 1.434(4) . . no
C30 C31 1.454(4) . . no
C31 C48 1.444(4) . . no
C31 C32 1.389(3) . . no
C32 C33 1.449(3) . . no
C33 C34 1.446(4) . . no
C33 C50 1.395(4) . . no
C34 C35 1.381(4) . . no
C35 C52 1.450(4) . . no
C35 C36 1.455(4) . . no
C36 C37 1.443(4) . . no
C37 C38 1.397(4) . . no
C37 C53 1.450(4) . . no
C38 C39 1.451(4) . . no
C39 C40 1.392(4) . . no
C40 C54 1.450(4) . . no
C40 C41 1.456(4) . . no
C41 C42 1.393(4) . . no
C41 C60 1.447(3) . . no
C42 C43 1.453(4) . . no
C43 C44 1.387(4) . . no
C44 C59 1.453(4) . . no
C44 C45 1.445(4) . . no
C45 C46 1.459(4) . . no
C46 C58 1.448(4) . . no
C46 C47 1.381(4) . . no
C47 C48 1.452(4) . . no
C48 C49 1.392(3) . . no
C49 C50 1.451(4) . . no
C49 C57 1.449(4) . . no
C50 C51 1.452(3) . . no
C51 C56 1.448(4) . . no
C51 C52 1.388(4) . . no
C52 C53 1.455(4) . . no

C53 C54 1.382(4) . . no
 C54 C55 1.455(3) . . no
 C55 C60 1.447(4) . . no
 C55 C56 1.384(4) . . no
 C56 C57 1.454(3) . . no
 C57 C58 1.390(4) . . no
 C58 C59 1.464(4) . . no
 C59 C60 1.390(4) . . no
 C61 C62 1.502(3) . . no
 C61 C68 1.533(4) . . no
 C62 C63 1.394(4) . . no
 C62 C67 1.394(4) . . no
 C63 C64 1.394(4) . . no
 C64 C65 1.383(4) . . no
 C65 C66 1.385(4) . . no
 C66 C67 1.388(4) . . no
 C68 C69 1.527(4) . . no
 C69 C70 1.537(4) . . no
 C70 C71 1.508(4) . . no
 C63 H63 1.02(2) . . no
 C64 H64 1.02(2) . . no
 C65 H65 1.01(2) . . no
 C66 H66 1.00(2) . . no
 C67 H67 1.03(2) . . no
 C68 H68' 1.09(2) . . no
 C68 H68 1.01(2) . . no
 C69 H69' 1.02(2) . . no
 C69 H69 1.06(2) . . no
 C70 H70' 1.02(2) . . no
 C70 H70 0.99(2) . . no
 C72 H72" 1.04(3) . . no
 C72 H72 0.96(2) . . no
 C72 H72' 1.07(3) . . no
 C73 C74 1.381(3) . . no
 C73 C78 1.384(4) . . no
 C74 C75 1.381(4) . . no
 C75 C76 1.387(4) . . no
 C76 C77 1.388(4) . . no
 C77 C78 1.382(4) . . no
 C75 H75 0.98(2) . . no
 C76 H76 0.97(2) . . no
 C77 H77 1.07(2) . . no
 C78 H78 1.04(2) . . no

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 C71 O2 C72 116.0(2) . . . yes
 C2 C1 C6 114.9(2) . . . no
 C2 C1 C9 114.74(19) . . . no
 C2 C1 C61 57.61(15) . . . no
 C6 C1 C9 105.4(2) . . . no
 C6 C1 C61 126.1(2) . . . no
 C9 C1 C61 126.8(2) . . . no
 C1 C2 C3 115.06(19) . . . no
 C1 C2 C12 115.0(2) . . . no
 C1 C2 C61 57.65(15) . . . no
 C3 C2 C12 104.81(19) . . . no
 C3 C2 C61 126.3(2) . . . no
 C12 C2 C61 127.1(2) . . . no
 C2 C3 C4 123.4(2) . . . no

C2 C3 C14 108.4(2) . . . no
C4 C3 C14 119.2(2) . . . no
C3 C4 C5 121.0(2) . . . no
C3 C4 C17 119.4(2) . . . no
C5 C4 C17 107.7(2) . . . no
C4 C5 C6 120.8(2) . . . no
C4 C5 C19 107.5(2) . . . no
C6 C5 C19 119.7(2) . . . no
C1 C6 C5 123.9(2) . . . no
C1 C6 C7 107.7(2) . . . no
C5 C6 C7 119.6(2) . . . no
C6 C7 C8 108.8(2) . . . no
C6 C7 C21 121.3(2) . . . no
C8 C7 C21 119.9(2) . . . no
C7 C8 C9 108.2(2) . . . no
C7 C8 C24 120.2(2) . . . no
C9 C8 C24 121.5(2) . . . no
C1 C9 C8 108.3(2) . . . no
C1 C9 C10 124.5(2) . . . no
C8 C9 C10 118.9(2) . . . no
C9 C10 C11 120.4(2) . . . no
C9 C10 C26 120.3(2) . . . no
C11 C10 C26 107.2(2) . . . no
C10 C11 C12 120.6(2) . . . no
C10 C11 C28 107.4(2) . . . no
C12 C11 C28 120.7(2) . . . no
C2 C12 C11 123.9(2) . . . no
C2 C12 C13 108.3(2) . . . no
C11 C12 C13 119.0(2) . . . no
C12 C13 C14 108.5(2) . . . no
C12 C13 C30 120.8(2) . . . no
C14 C13 C30 120.1(2) . . . no
C3 C14 C13 108.5(2) . . . no
C3 C14 C15 121.9(2) . . . no
C13 C14 C15 119.8(2) . . . no
C14 C15 C16 119.0(2) . . . no
C14 C15 C32 120.6(2) . . . no
C16 C15 C32 108.3(2) . . . no
C15 C16 C17 119.4(2) . . . no
C15 C16 C34 107.7(2) . . . no
C17 C16 C34 120.1(2) . . . no
C4 C17 C16 121.0(2) . . . no
C4 C17 C18 108.3(2) . . . no
C16 C17 C18 119.7(2) . . . no
C17 C18 C19 108.1(2) . . . no
C17 C18 C36 120.1(2) . . . no
C19 C18 C36 119.7(2) . . . no
C5 C19 C18 108.4(2) . . . no
C5 C19 C20 120.3(2) . . . no
C18 C19 C20 120.1(2) . . . no
C19 C20 C21 120.1(2) . . . no
C19 C20 C38 120.3(2) . . . no
C21 C20 C38 107.2(2) . . . no
C7 C21 C20 118.9(2) . . . no
C7 C21 C22 120.1(2) . . . no
C20 C21 C22 109.1(2) . . . no
C21 C22 C23 119.8(2) . . . no
C21 C22 C39 107.6(2) . . . no
C23 C22 C39 120.3(2) . . . no
C22 C23 C24 120.5(2) . . . no
C22 C23 C42 120.0(2) . . . no
C24 C23 C42 107.6(2) . . . no
C8 C24 C23 119.5(2) . . . no
C8 C24 C25 119.2(2) . . . no
C23 C24 C25 108.7(2) . . . no
C24 C25 C26 119.8(2) . . . no
C24 C25 C43 107.9(2) . . . no

C26	C25	C43	119.8(2)	.	.	.	no
C10	C26	C25	120.2(2)	.	.	.	no
C10	C26	C27	108.5(2)	.	.	.	no
C25	C26	C27	120.0(2)	.	.	.	no
C26	C27	C28	108.0(2)	.	.	.	no
C26	C27	C45	120.0(2)	.	.	.	no
C28	C27	C45	120.6(2)	.	.	.	no
C11	C28	C27	108.9(2)	.	.	.	no
C11	C28	C29	119.9(2)	.	.	.	no
C27	C28	C29	119.9(2)	.	.	.	no
C28	C29	C30	119.6(2)	.	.	.	no
C28	C29	C47	119.4(2)	.	.	.	no
C30	C29	C47	108.7(2)	.	.	.	no
C13	C30	C29	119.8(2)	.	.	.	no
C13	C30	C31	120.1(2)	.	.	.	no
C29	C30	C31	107.9(2)	.	.	.	no
C30	C31	C32	119.7(2)	.	.	.	no
C30	C31	C48	107.9(2)	.	.	.	no
C32	C31	C48	120.3(2)	.	.	.	no
C15	C32	C31	119.8(2)	.	.	.	no
C15	C32	C33	107.8(2)	.	.	.	no
C31	C32	C33	120.1(2)	.	.	.	no
C32	C33	C34	108.2(2)	.	.	.	no
C32	C33	C50	119.8(2)	.	.	.	no
C34	C33	C50	119.9(2)	.	.	.	no
C16	C34	C33	107.9(2)	.	.	.	no
C16	C34	C35	120.4(2)	.	.	.	no
C33	C34	C35	120.2(2)	.	.	.	no
C34	C35	C36	119.8(2)	.	.	.	no
C34	C35	C52	120.0(2)	.	.	.	no
C36	C35	C52	107.7(2)	.	.	.	no
C18	C36	C35	119.9(2)	.	.	.	no
C18	C36	C37	120.4(2)	.	.	.	no
C35	C36	C37	108.1(2)	.	.	.	no
C36	C37	C38	120.0(2)	.	.	.	no
C36	C37	C53	108.3(2)	.	.	.	no
C38	C37	C53	119.8(2)	.	.	.	no
C20	C38	C37	119.5(2)	.	.	.	no
C20	C38	C39	108.5(2)	.	.	.	no
C37	C38	C39	119.9(2)	.	.	.	no
C22	C39	C38	107.7(2)	.	.	.	no
C22	C39	C40	120.1(2)	.	.	.	no
C38	C39	C40	120.0(2)	.	.	.	no
C39	C40	C41	119.6(2)	.	.	.	no
C39	C40	C54	119.8(2)	.	.	.	no
C41	C40	C54	108.0(2)	.	.	.	no
C40	C41	C42	120.1(2)	.	.	.	no
C40	C41	C60	107.7(2)	.	.	.	no
C42	C41	C60	120.2(2)	.	.	.	no
C23	C42	C41	119.9(2)	.	.	.	no
C23	C42	C43	107.8(2)	.	.	.	no
C41	C42	C43	120.2(2)	.	.	.	no
C25	C43	C42	108.0(2)	.	.	.	no
C25	C43	C44	120.1(2)	.	.	.	no
C42	C43	C44	119.7(2)	.	.	.	no
C43	C44	C45	120.2(2)	.	.	.	no
C43	C44	C59	119.9(2)	.	.	.	no
C45	C44	C59	108.0(2)	.	.	.	no
C27	C45	C44	120.0(2)	.	.	.	no
C27	C45	C46	119.6(2)	.	.	.	no
C44	C45	C46	108.4(2)	.	.	.	no
C45	C46	C47	119.9(2)	.	.	.	no
C45	C46	C58	107.9(2)	.	.	.	no
C47	C46	C58	120.2(2)	.	.	.	no
C29	C47	C46	120.6(2)	.	.	.	no
C29	C47	C48	107.0(2)	.	.	.	no
C46	C47	C48	119.9(2)	.	.	.	no

C31	C48	C47	108.4(2)	.	.	.	no
C31	C48	C49	119.8(2)	.	.	.	no
C47	C48	C49	119.9(2)	.	.	.	no
C48	C49	C50	120.1(2)	.	.	.	no
C48	C49	C57	120.2(2)	.	.	.	no
C50	C49	C57	107.9(2)	.	.	.	no
C33	C50	C49	119.9(2)	.	.	.	no
C33	C50	C51	120.0(2)	.	.	.	no
C49	C50	C51	108.0(2)	.	.	.	no
C50	C51	C52	119.5(2)	.	.	.	no
C50	C51	C56	108.0(2)	.	.	.	no
C52	C51	C56	120.1(2)	.	.	.	no
C35	C52	C51	120.3(2)	.	.	.	no
C35	C52	C53	108.2(2)	.	.	.	no
C51	C52	C53	119.8(2)	.	.	.	no
C37	C53	C52	107.7(2)	.	.	.	no
C37	C53	C54	120.1(2)	.	.	.	no
C52	C53	C54	119.8(2)	.	.	.	no
C40	C54	C53	120.3(2)	.	.	.	no
C40	C54	C55	108.0(2)	.	.	.	no
C53	C54	C55	120.4(2)	.	.	.	no
C54	C55	C56	119.6(2)	.	.	.	no
C54	C55	C60	107.7(2)	.	.	.	no
C56	C55	C60	120.7(2)	.	.	.	no
C51	C56	C55	120.3(2)	.	.	.	no
C51	C56	C57	107.9(2)	.	.	.	no
C55	C56	C57	119.7(2)	.	.	.	no
C49	C57	C56	108.1(2)	.	.	.	no
C49	C57	C58	119.5(2)	.	.	.	no
C56	C57	C58	120.3(2)	.	.	.	no
C46	C58	C57	120.3(2)	.	.	.	no
C46	C58	C59	107.8(2)	.	.	.	no
C57	C58	C59	119.6(2)	.	.	.	no
C44	C59	C58	107.9(2)	.	.	.	no
C44	C59	C60	120.6(2)	.	.	.	no
C58	C59	C60	119.9(2)	.	.	.	no
C41	C60	C55	108.6(2)	.	.	.	no
C41	C60	C59	119.5(2)	.	.	.	no
C55	C60	C59	119.9(2)	.	.	.	no
C1	C61	C2	64.74(16)	.	.	.	no
C1	C61	C62	117.04(19)	.	.	.	no
C1	C61	C68	116.4(2)	.	.	.	no
C2	C61	C62	117.5(2)	.	.	.	no
C2	C61	C68	116.57(19)	.	.	.	no
C62	C61	C68	115.3(2)	.	.	.	no
C61	C62	C63	120.0(2)	.	.	.	no
C61	C62	C67	121.1(2)	.	.	.	no
C63	C62	C67	118.9(2)	.	.	.	no
C62	C63	C64	120.6(3)	.	.	.	no
C63	C64	C65	119.8(3)	.	.	.	no
C64	C65	C66	120.1(3)	.	.	.	no
C65	C66	C67	120.2(3)	.	.	.	no
C62	C67	C66	120.5(2)	.	.	.	no
C61	C68	C69	114.4(2)	.	.	.	no
C68	C69	C70	110.9(2)	.	.	.	no
C69	C70	C71	112.0(2)	.	.	.	no
O1	C71	O2	123.3(2)	.	.	.	yes
O1	C71	C70	125.0(3)	.	.	.	yes
O2	C71	C70	111.6(2)	.	.	.	yes
C62	C63	H63	117.7(13)	.	.	.	no
C64	C63	H63	121.7(13)	.	.	.	no
C63	C64	H64	119.0(12)	.	.	.	no
C65	C64	H64	121.1(12)	.	.	.	no
C64	C65	H65	119.5(12)	.	.	.	no
C66	C65	H65	120.3(12)	.	.	.	no
C65	C66	H66	122.4(12)	.	.	.	no
C67	C66	H66	117.4(12)	.	.	.	no

C62 C67 H67 124.7(13) . . . no
 C66 C67 H67 114.8(13) . . . no
 C61 C68 H68 107.7(12) . . . no
 C61 C68 H68' 108.1(11) . . . no
 C69 C68 H68 108.7(12) . . . no
 C69 C68 H68' 110.2(11) . . . no
 H68 C68 H68' 107.6(17) . . . no
 C68 C69 H69 111.3(12) . . . no
 C68 C69 H69' 108.9(11) . . . no
 C70 C69 H69 106.9(12) . . . no
 C70 C69 H69' 110.5(11) . . . no
 H69 C69 H69' 108.3(16) . . . no
 C69 C70 H70 110.8(13) . . . no
 C69 C70 H70' 112.5(14) . . . no
 C71 C70 H70 108.4(14) . . . no
 C71 C70 H70' 104.9(14) . . . no
 H70 C70 H70' 108.0(19) . . . no
 O2 C72 H72 110.7(14) . . . no
 O2 C72 H72' 107.1(16) . . . no
 O2 C72 H72" 103.0(16) . . . no
 H72 C72 H72' 109(2) . . . no
 H72 C72 H72" 111.6(19) . . . no
 H72' C72 H72" 116(2) . . . no
 C11 C73 C74 121.1(2) . . . yes
 C11 C73 C78 118.83(19) . . . yes
 C74 C73 C78 120.0(2) . . . no
 C12 C74 C73 120.05(19) . . . yes
 C12 C74 C75 119.2(2) . . . yes
 C73 C74 C75 120.8(2) . . . no
 C74 C75 C76 119.3(3) . . . no
 C75 C76 C77 119.9(3) . . . no
 C76 C77 C78 120.4(3) . . . no
 C73 C78 C77 119.5(2) . . . no
 C74 C75 H75 122.4(14) . . . no
 C76 C75 H75 118.1(14) . . . no
 C75 C76 H76 118.5(13) . . . no
 C77 C76 H76 121.5(13) . . . no
 C76 C77 H77 119.3(11) . . . no
 C78 C77 H77 120.3(11) . . . no
 C73 C78 H78 119.1(13) . . . no
 C77 C78 H78 121.3(13) . . . no

loop_

_geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
 C72 O2 C71 O1 2.9(3) no
 C72 O2 C71 C70 -178.1(2) no
 C6 C1 C2 C12 122.2(2) no
 C9 C1 C2 C12 -0.2(3) no
 C6 C1 C2 C61 -118.3(2) no
 C9 C1 C2 C3 -122.2(2) no
 C6 C1 C2 C3 0.2(3) no
 C2 C1 C6 C5 7.5(3) no
 C2 C1 C6 C7 -139.6(2) no
 C9 C1 C6 C5 134.9(3) no
 C9 C1 C6 C7 -12.3(3) no
 C9 C1 C2 C61 119.3(2) no
 C61 C1 C2 C3 118.5(2) no
 C61 C1 C2 C12 -119.5(2) no

C2 C1 C9 C10 -7.7(3) no
C6 C1 C9 C8 12.5(3) no
C6 C1 C9 C10 -135.2(2) no
C61 C1 C9 C8 -153.1(2) no
C61 C1 C9 C10 59.2(3) no
C2 C1 C61 C62 -109.4(2) no
C2 C1 C61 C68 108.5(2) no
C6 C1 C61 C2 98.9(3) no
C6 C1 C61 C62 -10.5(3) no
C6 C1 C61 C68 -152.6(2) no
C9 C1 C61 C2 -98.3(3) no
C9 C1 C61 C62 152.3(2) no
C61 C1 C6 C5 -59.4(4) no
C61 C1 C6 C7 153.5(2) no
C2 C1 C9 C8 140.0(2) no
C9 C1 C61 C68 10.2(3) no
C12 C2 C3 C14 11.6(3) no
C61 C2 C3 C4 59.3(3) no
C61 C2 C3 C14 -153.9(2) no
C1 C2 C12 C11 7.4(3) no
C1 C2 C12 C13 -139.4(2) no
C3 C2 C12 C11 134.8(2) no
C3 C2 C12 C13 -12.1(3) no
C61 C2 C12 C11 -59.8(4) no
C61 C2 C12 C13 153.3(2) no
C1 C2 C61 C62 108.7(2) no
C1 C2 C61 C68 -108.3(2) no
C3 C2 C61 C1 -99.0(3) no
C3 C2 C61 C62 9.7(3) no
C3 C2 C61 C68 152.7(2) no
C12 C2 C3 C4 -135.1(2) no
C12 C2 C61 C62 -152.7(2) no
C12 C2 C61 C68 -9.7(4) no
C1 C2 C3 C14 139.0(2) no
C12 C2 C61 C1 98.6(3) no
C1 C2 C3 C4 -7.7(3) no
C2 C3 C4 C17 146.2(2) no
C2 C3 C14 C13 -7.0(3) no
C14 C3 C4 C5 -135.4(2) no
C14 C3 C4 C17 2.8(3) no
C2 C3 C4 C5 8.0(4) no
C4 C3 C14 C15 -4.2(4) no
C2 C3 C14 C15 -152.6(2) no
C4 C3 C14 C13 141.4(2) no
C3 C4 C5 C6 0.1(4) no
C3 C4 C5 C19 142.6(2) no
C17 C4 C5 C6 -142.4(2) no
C17 C4 C5 C19 0.1(4) no
C5 C4 C17 C18 -0.7(3) no
C5 C4 C17 C16 143.2(2) no
C3 C4 C17 C16 0.0(4) no
C3 C4 C17 C18 -143.9(2) no
C4 C5 C6 C7 135.4(2) no
C4 C5 C19 C18 0.5(3) no
C19 C5 C6 C1 -146.1(2) no
C19 C5 C6 C7 -2.6(3) no
C4 C5 C6 C1 -8.1(4) no
C6 C5 C19 C20 -0.2(4) no
C4 C5 C19 C20 -143.2(2) no
C6 C5 C19 C18 143.4(2) no
C1 C6 C7 C8 7.6(3) no
C1 C6 C7 C21 152.9(2) no
C5 C6 C7 C8 -141.2(2) no
C5 C6 C7 C21 4.1(3) no
C21 C7 C8 C24 0.2(4) no
C6 C7 C21 C20 -2.5(3) no
C6 C7 C21 C22 -141.2(2) no

C8 C7 C21 C20 139.1(2) no
C8 C7 C21 C22 0.4(4) no
C6 C7 C8 C9 0.3(3) no
C6 C7 C8 C24 146.0(2) no
C21 C7 C8 C9 -145.5(2) no
C24 C8 C9 C10 -3.6(4) no
C7 C8 C24 C23 -0.8(4) no
C7 C8 C24 C25 -138.4(2) no
C9 C8 C24 C23 140.3(2) no
C7 C8 C9 C1 -8.2(3) no
C7 C8 C9 C10 141.6(2) no
C24 C8 C9 C1 -153.3(2) no
C9 C8 C24 C25 2.6(4) no
C8 C9 C10 C26 1.9(4) no
C1 C9 C10 C26 146.4(2) no
C8 C9 C10 C11 -135.8(2) no
C1 C9 C10 C11 8.8(4) no
C9 C10 C11 C28 142.8(2) no
C9 C10 C26 C25 0.7(4) no
C26 C10 C11 C12 -143.6(2) no
C26 C10 C11 C28 0.3(3) no
C9 C10 C11 C12 -1.0(4) no
C11 C10 C26 C27 -0.3(3) no
C9 C10 C26 C27 -142.9(2) no
C11 C10 C26 C25 143.2(2) no
C10 C11 C12 C2 -7.2(4) no
C10 C11 C12 C13 136.4(2) no
C28 C11 C12 C2 -146.4(2) no
C28 C11 C12 C13 -2.8(3) no
C12 C11 C28 C29 0.1(4) no
C12 C11 C28 C27 143.6(2) no
C10 C11 C28 C27 -0.2(3) no
C10 C11 C28 C29 -143.8(2) no
C2 C12 C13 C14 8.2(3) no
C2 C12 C13 C30 152.8(2) no
C11 C12 C13 C14 -140.6(2) no
C11 C12 C13 C30 4.0(3) no
C30 C13 C14 C15 0.9(4) no
C12 C13 C30 C29 -2.5(3) no
C12 C13 C30 C31 -140.5(2) no
C14 C13 C30 C29 138.0(2) no
C12 C13 C14 C3 -0.7(3) no
C12 C13 C14 C15 145.7(2) no
C30 C13 C14 C3 -145.6(2) no
C14 C13 C30 C31 0.0(4) no
C13 C14 C15 C32 -1.3(4) no
C3 C14 C15 C32 140.6(2) no
C13 C14 C15 C16 -139.3(2) no
C3 C14 C15 C16 2.6(4) no
C14 C15 C16 C17 0.4(4) no
C14 C15 C16 C34 142.0(2) no
C32 C15 C16 C17 -142.3(2) no
C32 C15 C16 C34 -0.7(3) no
C16 C15 C32 C33 0.4(3) no
C14 C15 C32 C31 0.8(4) no
C14 C15 C32 C33 -141.6(2) no
C16 C15 C32 C31 142.7(2) no
C15 C16 C17 C4 -1.7(4) no
C15 C16 C17 C18 138.2(3) no
C34 C16 C17 C4 -138.5(2) no
C17 C16 C34 C33 142.0(2) no
C17 C16 C34 C35 -1.3(4) no
C34 C16 C17 C18 1.4(4) no
C15 C16 C34 C33 0.8(3) no
C15 C16 C34 C35 -142.6(2) no
C4 C17 C18 C19 1.0(3) no
C4 C17 C18 C36 143.3(2) no

C16 C17 C18 C19 -143.5(2) no
C16 C17 C18 C36 -1.1(4) no
C36 C18 C19 C5 -143.4(2) no
C17 C18 C36 C35 0.8(4) no
C17 C18 C36 C37 -138.1(3) no
C36 C18 C19 C20 0.4(4) no
C17 C18 C19 C5 -0.9(3) no
C17 C18 C19 C20 142.9(2) no
C19 C18 C36 C37 -0.1(4) no
C19 C18 C36 C35 138.8(2) no
C18 C19 C20 C38 -0.4(3) no
C5 C19 C20 C21 1.8(3) no
C5 C19 C20 C38 139.0(2) no
C18 C19 C20 C21 -137.7(2) no
C38 C20 C21 C7 -142.6(2) no
C19 C20 C21 C22 142.4(2) no
C19 C20 C38 C39 -142.2(2) no
C38 C20 C21 C22 0.3(3) no
C19 C20 C38 C37 0.2(3) no
C19 C20 C21 C7 -0.4(3) no
C21 C20 C38 C37 142.3(2) no
C21 C20 C38 C39 -0.1(2) no
C7 C21 C22 C39 142.0(2) no
C7 C21 C22 C23 -0.2(4) no
C20 C21 C22 C23 -142.6(2) no
C20 C21 C22 C39 -0.3(3) no
C21 C22 C23 C24 -0.4(4) no
C21 C22 C39 C38 0.2(3) no
C21 C22 C39 C40 -142.2(2) no
C23 C22 C39 C38 142.3(2) no
C23 C22 C39 C40 -0.1(4) no
C39 C22 C23 C42 0.2(4) no
C21 C22 C23 C42 137.8(2) no
C39 C22 C23 C24 -137.9(3) no
C22 C23 C24 C8 0.9(4) no
C22 C23 C42 C41 -0.3(4) no
C22 C23 C42 C43 -142.7(2) no
C24 C23 C42 C41 142.6(2) no
C24 C23 C42 C43 0.2(3) no
C22 C23 C24 C25 142.5(2) no
C42 C23 C24 C8 -141.8(2) no
C42 C23 C24 C25 -0.2(3) no
C23 C24 C25 C43 0.1(3) no
C23 C24 C25 C26 -141.8(2) no
C8 C24 C25 C26 0.0(4) no
C8 C24 C25 C43 141.9(2) no
C24 C25 C26 C27 137.8(3) no
C24 C25 C43 C42 0.0(3) no
C43 C25 C26 C10 -139.1(2) no
C43 C25 C26 C27 0.3(4) no
C24 C25 C26 C10 -1.6(4) no
C26 C25 C43 C44 -0.3(4) no
C24 C25 C43 C44 -142.3(2) no
C26 C25 C43 C42 142.0(2) no
C10 C26 C27 C28 0.2(3) no
C10 C26 C27 C45 143.9(2) no
C25 C26 C27 C28 -143.4(2) no
C25 C26 C27 C45 0.3(4) no
C45 C27 C28 C29 0.1(4) no
C26 C27 C45 C44 -0.9(4) no
C26 C27 C45 C46 -139.0(2) no
C28 C27 C45 C44 138.3(3) no
C28 C27 C45 C46 0.2(4) no
C26 C27 C28 C11 0.0(3) no
C26 C27 C28 C29 143.6(2) no
C45 C27 C28 C11 -143.5(2) no
C27 C28 C29 C47 -0.1(3) no

C11	C28	C29	C30	1.5(4)	.	.	.	.	no
C11	C28	C29	C47	139.5(2)	.	.	.	.	no
C27	C28	C29	C30	-138.1(2)	.	.	.	.	no
C28	C29	C30	C13	-0.2(4)	.	.	.	.	no
C28	C29	C30	C31	142.3(2)	.	.	.	.	no
C47	C29	C30	C13	-142.3(2)	.	.	.	.	no
C30	C29	C47	C46	141.9(2)	.	.	.	.	no
C30	C29	C47	C48	0.0(2)	.	.	.	.	no
C28	C29	C47	C48	-142.1(2)	.	.	.	.	no
C47	C29	C30	C31	0.2(3)	.	.	.	.	no
C28	C29	C47	C46	-0.3(4)	.	.	.	.	no
C13	C30	C31	C48	142.0(2)	.	.	.	.	no
C13	C30	C31	C32	-0.5(4)	.	.	.	.	no
C29	C30	C31	C32	-143.0(2)	.	.	.	.	no
C29	C30	C31	C48	-0.4(2)	.	.	.	.	no
C30	C31	C32	C15	0.1(4)	.	.	.	.	no
C30	C31	C48	C47	0.4(2)	.	.	.	.	no
C30	C31	C48	C49	-142.5(2)	.	.	.	.	no
C32	C31	C48	C47	142.7(2)	.	.	.	.	no
C32	C31	C48	C49	-0.2(4)	.	.	.	.	no
C30	C31	C32	C33	137.9(2)	.	.	.	.	no
C48	C31	C32	C15	-137.8(2)	.	.	.	.	no
C48	C31	C32	C33	-0.1(4)	.	.	.	.	no
C31	C32	C33	C50	0.3(4)	.	.	.	.	no
C31	C32	C33	C34	-142.1(2)	.	.	.	.	no
C15	C32	C33	C34	0.1(3)	.	.	.	.	no
C15	C32	C33	C50	142.5(2)	.	.	.	.	no
C32	C33	C34	C16	-0.5(3)	.	.	.	.	no
C32	C33	C34	C35	142.9(2)	.	.	.	.	no
C50	C33	C34	C16	-142.9(2)	.	.	.	.	no
C50	C33	C34	C35	0.5(4)	.	.	.	.	no
C34	C33	C50	C51	-0.4(4)	.	.	.	.	no
C32	C33	C50	C49	-0.3(4)	.	.	.	.	no
C32	C33	C50	C51	-138.5(2)	.	.	.	.	no
C34	C33	C50	C49	137.8(2)	.	.	.	.	no
C16	C34	C35	C36	1.0(4)	.	.	.	.	no
C16	C34	C35	C52	138.3(3)	.	.	.	.	no
C33	C34	C35	C36	-137.9(3)	.	.	.	.	no
C33	C34	C35	C52	-0.6(4)	.	.	.	.	no
C52	C35	C36	C37	0.7(3)	.	.	.	.	no
C34	C35	C52	C51	0.5(4)	.	.	.	.	no
C52	C35	C36	C18	-142.7(2)	.	.	.	.	no
C36	C35	C52	C51	142.4(2)	.	.	.	.	no
C36	C35	C52	C53	-0.6(3)	.	.	.	.	no
C34	C35	C52	C53	-142.5(2)	.	.	.	.	no
C34	C35	C36	C18	-0.7(4)	.	.	.	.	no
C34	C35	C36	C37	142.7(2)	.	.	.	.	no
C35	C36	C37	C53	-0.5(3)	.	.	.	.	no
C18	C36	C37	C38	-0.1(4)	.	.	.	.	no
C18	C36	C37	C53	142.7(2)	.	.	.	.	no
C35	C36	C37	C38	-143.3(2)	.	.	.	.	no
C36	C37	C38	C20	0.0(4)	.	.	.	.	no
C36	C37	C38	C39	138.2(2)	.	.	.	.	no
C53	C37	C38	C20	-138.5(2)	.	.	.	.	no
C38	C37	C53	C52	143.0(2)	.	.	.	.	no
C38	C37	C53	C54	1.0(4)	.	.	.	.	no
C53	C37	C38	C39	-0.4(4)	.	.	.	.	no
C36	C37	C53	C52	0.1(3)	.	.	.	.	no
C36	C37	C53	C54	-141.8(2)	.	.	.	.	no
C20	C38	C39	C22	0.0(3)	.	.	.	.	no
C20	C38	C39	C40	142.4(2)	.	.	.	.	no
C37	C38	C39	C22	-142.3(2)	.	.	.	.	no
C37	C38	C39	C40	0.1(4)	.	.	.	.	no
C38	C39	C40	C41	-137.8(2)	.	.	.	.	no
C22	C39	C40	C41	0.0(4)	.	.	.	.	no
C22	C39	C40	C54	137.3(3)	.	.	.	.	no
C38	C39	C40	C54	-0.4(4)	.	.	.	.	no

C39	C40	C41	C42	-0.1(4)	.	.	.	.	no
C39	C40	C41	C60	142.5(2)	.	.	.	.	no
C39	C40	C54	C55	-142.6(2)	.	.	.	.	no
C41	C40	C54	C53	142.9(2)	.	.	.	.	no
C41	C40	C54	C55	-0.9(3)	.	.	.	.	no
C39	C40	C54	C53	1.1(4)	.	.	.	.	no
C54	C40	C41	C42	-141.9(2)	.	.	.	.	no
C54	C40	C41	C60	0.7(3)	.	.	.	.	no
C40	C41	C42	C43	138.0(2)	.	.	.	.	no
C40	C41	C60	C55	-0.2(3)	.	.	.	.	no
C60	C41	C42	C23	-137.8(2)	.	.	.	.	no
C60	C41	C42	C43	0.1(4)	.	.	.	.	no
C40	C41	C42	C23	0.2(4)	.	.	.	.	no
C42	C41	C60	C59	-0.2(4)	.	.	.	.	no
C40	C41	C60	C59	-142.8(2)	.	.	.	.	no
C42	C41	C60	C55	142.3(2)	.	.	.	.	no
C23	C42	C43	C25	-0.1(3)	.	.	.	.	no
C23	C42	C43	C44	142.3(2)	.	.	.	.	no
C41	C42	C43	C25	-142.4(2)	.	.	.	.	no
C41	C42	C43	C44	0.0(4)	.	.	.	.	no
C42	C43	C44	C59	0.1(4)	.	.	.	.	no
C42	C43	C44	C45	-138.2(3)	.	.	.	.	no
C25	C43	C44	C45	-0.2(4)	.	.	.	.	no
C25	C43	C44	C59	138.0(3)	.	.	.	.	no
C43	C44	C45	C27	0.8(4)	.	.	.	.	no
C43	C44	C45	C46	143.1(2)	.	.	.	.	no
C59	C44	C45	C27	-141.8(2)	.	.	.	.	no
C59	C44	C45	C46	0.5(3)	.	.	.	.	no
C45	C44	C59	C60	142.5(2)	.	.	.	.	no
C43	C44	C59	C58	-143.3(2)	.	.	.	.	no
C43	C44	C59	C60	-0.2(4)	.	.	.	.	no
C45	C44	C59	C58	-0.5(3)	.	.	.	.	no
C27	C45	C46	C47	-0.5(4)	.	.	.	.	no
C27	C45	C46	C58	142.2(2)	.	.	.	.	no
C44	C45	C46	C47	-143.0(2)	.	.	.	.	no
C44	C45	C46	C58	-0.3(3)	.	.	.	.	no
C58	C46	C47	C48	-0.5(4)	.	.	.	.	no
C45	C46	C58	C57	-142.1(2)	.	.	.	.	no
C58	C46	C47	C29	-137.6(2)	.	.	.	.	no
C47	C46	C58	C57	0.4(4)	.	.	.	.	no
C47	C46	C58	C59	142.5(2)	.	.	.	.	no
C45	C46	C58	C59	0.0(3)	.	.	.	.	no
C45	C46	C47	C29	0.5(4)	.	.	.	.	no
C45	C46	C47	C48	137.6(2)	.	.	.	.	no
C46	C47	C48	C49	0.4(3)	.	.	.	.	no
C29	C47	C48	C31	-0.3(2)	.	.	.	.	no
C29	C47	C48	C49	142.6(2)	.	.	.	.	no
C46	C47	C48	C31	-142.4(2)	.	.	.	.	no
C31	C48	C49	C50	0.2(4)	.	.	.	.	no
C31	C48	C49	C57	138.5(2)	.	.	.	.	no
C47	C48	C49	C50	-138.5(2)	.	.	.	.	no
C47	C48	C49	C57	-0.2(4)	.	.	.	.	no
C57	C49	C50	C33	-142.8(2)	.	.	.	.	no
C57	C49	C50	C51	-0.1(3)	.	.	.	.	no
C48	C49	C57	C58	0.1(4)	.	.	.	.	no
C50	C49	C57	C56	0.2(3)	.	.	.	.	no
C48	C49	C57	C56	-142.6(2)	.	.	.	.	no
C48	C49	C50	C33	0.0(4)	.	.	.	.	no
C48	C49	C50	C51	142.7(2)	.	.	.	.	no
C50	C49	C57	C58	142.9(2)	.	.	.	.	no
C49	C50	C51	C52	-142.2(2)	.	.	.	.	no
C33	C50	C51	C52	0.3(4)	.	.	.	.	no
C33	C50	C51	C56	142.6(2)	.	.	.	.	no
C49	C50	C51	C56	0.0(3)	.	.	.	.	no
C50	C51	C52	C35	-0.4(4)	.	.	.	.	no
C50	C51	C52	C53	138.4(3)	.	.	.	.	no
C50	C51	C56	C57	0.1(3)	.	.	.	.	no

C52	C51	C56	C55	-0.2(4)	.	.	.	.	no
C52	C51	C56	C57	142.1(2)	.	.	.	.	no
C50	C51	C56	C55	-142.2(2)	.	.	.	.	no
C56	C51	C52	C35	-138.1(3)	.	.	.	.	no
C56	C51	C52	C53	0.7(4)	.	.	.	.	no
C35	C52	C53	C37	0.3(3)	.	.	.	.	no
C35	C52	C53	C54	142.4(2)	.	.	.	.	no
C51	C52	C53	C37	-143.0(2)	.	.	.	.	no
C51	C52	C53	C54	-0.8(4)	.	.	.	.	no
C52	C53	C54	C55	0.5(4)	.	.	.	.	no
C37	C53	C54	C40	-1.4(4)	.	.	.	.	no
C37	C53	C54	C55	137.9(2)	.	.	.	.	no
C52	C53	C54	C40	-138.9(2)	.	.	.	.	no
C40	C54	C55	C56	143.7(2)	.	.	.	.	no
C40	C54	C55	C60	0.8(3)	.	.	.	.	no
C53	C54	C55	C56	0.0(4)	.	.	.	.	no
C53	C54	C55	C60	-143.0(2)	.	.	.	.	no
C60	C55	C56	C51	138.0(3)	.	.	.	.	no
C60	C55	C56	C57	0.0(4)	.	.	.	.	no
C54	C55	C60	C59	142.1(2)	.	.	.	.	no
C56	C55	C60	C41	-142.8(2)	.	.	.	.	no
C54	C55	C60	C41	-0.4(3)	.	.	.	.	no
C54	C55	C56	C51	-0.1(4)	.	.	.	.	no
C54	C55	C56	C57	-138.1(3)	.	.	.	.	no
C56	C55	C60	C59	-0.4(4)	.	.	.	.	no
C55	C56	C57	C49	142.4(2)	.	.	.	.	no
C51	C56	C57	C49	-0.2(3)	.	.	.	.	no
C51	C56	C57	C58	-142.5(2)	.	.	.	.	no
C55	C56	C57	C58	0.1(4)	.	.	.	.	no
C49	C57	C58	C46	-0.2(4)	.	.	.	.	no
C49	C57	C58	C59	-137.9(2)	.	.	.	.	no
C56	C57	C58	C59	0.2(4)	.	.	.	.	no
C56	C57	C58	C46	137.9(2)	.	.	.	.	no
C57	C58	C59	C44	142.7(2)	.	.	.	.	no
C57	C58	C59	C60	-0.6(4)	.	.	.	.	no
C46	C58	C59	C60	-143.0(2)	.	.	.	.	no
C46	C58	C59	C44	0.4(3)	.	.	.	.	no
C44	C59	C60	C41	0.3(4)	.	.	.	.	no
C44	C59	C60	C55	-138.1(3)	.	.	.	.	no
C58	C59	C60	C41	139.1(3)	.	.	.	.	no
C58	C59	C60	C55	0.7(4)	.	.	.	.	no
C2	C61	C62	C63	-123.3(2)	.	.	.	.	no
C68	C61	C62	C63	93.2(3)	.	.	.	.	no
C68	C61	C62	C67	-84.2(3)	.	.	.	.	no
C2	C61	C62	C67	59.2(3)	.	.	.	.	no
C1	C61	C62	C63	-49.3(3)	.	.	.	.	no
C1	C61	C62	C67	133.3(2)	.	.	.	.	no
C62	C61	C68	C69	78.8(3)	.	.	.	.	no
C1	C61	C68	C69	-138.5(2)	.	.	.	.	no
C2	C61	C68	C69	-65.0(3)	.	.	.	.	no
C67	C62	C63	C64	-0.4(4)	.	.	.	.	no
C61	C62	C63	C64	-177.9(2)	.	.	.	.	no
C61	C62	C67	C66	177.0(2)	.	.	.	.	no
C63	C62	C67	C66	-0.4(4)	.	.	.	.	no
C62	C63	C64	C65	0.7(4)	.	.	.	.	no
C63	C64	C65	C66	-0.2(4)	.	.	.	.	no
C64	C65	C66	C67	-0.6(4)	.	.	.	.	no
C65	C66	C67	C62	0.9(4)	.	.	.	.	no
C61	C68	C69	C70	174.8(2)	.	.	.	.	no
C68	C69	C70	C71	-61.0(3)	.	.	.	.	no
C69	C70	C71	O1	-37.1(4)	.	.	.	.	no
C69	C70	C71	O2	143.8(2)	.	.	.	.	no
C11	C73	C74	C12	0.6(3)	.	.	.	.	no
C11	C73	C74	C75	-179.5(2)	.	.	.	.	no
C78	C73	C74	C12	179.7(2)	.	.	.	.	no
C78	C73	C74	C75	-0.4(4)	.	.	.	.	no
C11	C73	C78	C77	178.5(2)	.	.	.	.	no

C74 C73 C78 C77 -0.7(4) no
 C12 C74 C75 C76 -179.2(2) no
 C73 C74 C75 C76 0.8(4) no
 C74 C75 C76 C77 -0.3(4) no
 C75 C76 C77 C78 -0.8(4) no
 C76 C77 C78 C73 1.2(4) 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

C11 C72 3.649(3) . . no
 C11 C10 3.489(3) . . no
 C11 C12 3.1516(9) . . no
 C11 C9 3.552(2) . . no
 C12 C11 3.1516(9) . . no
 C12 C9 3.644(2) . . no
 C12 C29 3.360(2) . 4_555 no
 C11 H72' 2.71(3) . . no
 C12 H63 2.98(2) . . no
 C12 H68' 3.00(2) . . no
 C12 H65 2.90(2) . 3_656 no
 O1 C11 3.092(3) . . no
 O1 C68 3.293(3) . . no
 O1 C66 3.409(3) . 2_555 no
 O2 C51 3.225(3) . 1_655 no
 O2 C56 3.236(3) . 1_655 no
 O2 C50 3.394(3) . 1_655 no
 O2 C38 3.197(3) . 4_554 no
 O2 C57 3.408(3) . 1_655 no
 O1 H68 2.70(2) . . no
 O1 H72' 2.75(3) . . no
 O1 H69 2.69(2) . . no
 O1 H72 2.50(2) . . no
 O1 H66 2.52(2) . 2_555 no
 O1 H75 2.75(2) . 4_454 no
 C3 C72 3.516(4) . 2_545 no
 C3 C67 3.313(4) . . no
 C4 C62 3.410(3) . . no
 C5 C62 3.405(4) . . no
 C5 C63 3.530(4) . . no
 C6 C63 3.135(4) . . no
 C7 C48 3.360(3) . 4_555 no
 C9 C12 3.644(2) . . no
 C9 C11 3.552(2) . . no
 C10 C68 3.416(4) . . no
 C10 C11 3.489(3) . . no
 C11 O1 3.092(3) . . no
 C11 C68 3.429(4) . . no
 C12 C69 3.369(4) . . no
 C16 C58 3.433(4) . 2_445 no
 C17 C18 3.582(4) . 3_556 no
 C18 C17 3.582(4) . 3_556 no
 C20 C72 3.448(4) . 4_455 no
 C21 C48 3.277(3) . 4_555 no
 C21 C49 3.359(3) . 4_555 no
 C23 C42 3.504(4) . 3_566 no
 C23 C41 3.468(4) . 3_566 no
 C24 C77 3.495(4) . 3_666 no
 C29 C12 3.360(2) . 4_454 no
 C32 C60 3.406(4) . 2_445 no
 C32 C59 3.403(4) . 2_445 no
 C33 C59 3.171(4) . 2_445 no
 C34 C58 3.454(4) . 2_445 no

C34 C59 3.316(4) . 2_445 no
C35 C65 3.392(4) . 3_556 no
C35 C64 3.594(4) . 3_556 no
C36 C65 3.513(4) . 3_556 no
C38 C72 3.363(4) . 4_455 no
C38 C71 3.378(3) . 4_455 no
C38 O2 3.197(3) . 4_455 no
C40 C76 3.483(4) . 1_455 no
C41 C23 3.468(4) . 3_566 no
C42 C23 3.504(4) . 3_566 no
C42 C42 3.554(3) . 3_566 no
C43 C70 3.547(4) . 2_555 no
C48 C7 3.360(3) . 4_454 no
C48 C21 3.277(3) . 4_454 no
C49 C21 3.359(3) . 4_454 no
C50 O2 3.394(3) . 1_455 no
C51 O2 3.225(3) . 1_455 no
C52 C65 3.560(4) . 3_556 no
C54 C76 3.420(4) . 1_455 no
C54 C75 3.485(4) . 1_455 no
C54 C77 3.506(4) . 1_455 no
C55 C78 3.504(4) . 1_455 no
C56 O2 3.236(3) . 1_455 no
C57 O2 3.408(3) . 1_455 no
C58 C34 3.454(4) . 2_455 no
C58 C16 3.433(4) . 2_455 no
C59 C34 3.316(4) . 2_455 no
C59 C32 3.403(4) . 2_455 no
C59 C33 3.171(4) . 2_455 no
C60 C32 3.406(4) . 2_455 no
C62 C5 3.405(4) . . no
C62 C4 3.410(3) . . no
C63 C64 3.581(4) . 3_656 no
C63 C6 3.135(4) . . no
C63 C65 3.523(4) . 3_656 no
C63 C5 3.530(4) . . no
C64 C35 3.594(4) . 3_556 no
C64 C63 3.581(4) . 3_656 no
C64 C65 3.594(4) . 3_656 no
C64 C64 3.379(4) . 3_656 no
C65 C35 3.392(4) . 3_556 no
C65 C63 3.523(4) . 3_656 no
C65 C36 3.513(4) . 3_556 no
C65 C64 3.594(4) . 3_656 no
C65 C52 3.560(4) . 3_556 no
C66 O1 3.409(3) . 2_545 no
C67 C69 3.501(4) . . no
C67 C3 3.313(4) . . no
C68 C11 3.429(4) . . no
C68 O1 3.293(3) . . no
C68 C10 3.416(4) . . no
C69 C67 3.501(4) . . no
C69 C12 3.369(4) . . no
C70 C43 3.547(4) . 2_545 no
C71 C38 3.378(3) . 4_554 no
C72 C11 3.649(3) . . no
C72 C3 3.516(4) . 2_555 no
C72 C38 3.363(4) . 4_554 no
C72 C20 3.448(4) . 4_554 no
C73 C77 3.420(4) . 3_666 no
C75 C54 3.485(4) . 1_655 no
C76 C54 3.420(4) . 1_655 no
C76 C40 3.483(4) . 1_655 no
C77 C24 3.495(4) . 3_666 no
C77 C73 3.420(4) . 3_666 no
C77 C54 3.506(4) . 1_655 no
C78 C55 3.504(4) . 1_655 no

C1 H63 2.81(2) . . no
C2 H67 3.08(2) . . no
C2 H69 2.89(2) . . no
C6 H63 2.76(2) . . no
C8 H77 2.90(2) . 3_666 no
C9 H68 2.56(2) . . no
C10 H68 2.63(2) . . no
C11 H68 2.81(2) . . no
C12 H69 2.71(2) . . no
C12 H68 2.91(2) . . no
C13 H78 2.75(2) . 2_545 no
C14 H78 3.02(2) . 2_545 no
C16 H72" 3.07(3) . 2_545 no
C24 H77 2.62(2) . 3_666 no
C25 H76 3.06(2) . 3_666 no
C26 H69' 3.09(2) . 2_555 no
C27 H69' 3.09(2) . 2_555 no
C28 H66 3.05(2) . 2_555 no
C30 H78 2.78(2) . 2_545 no
C31 H78 3.08(2) . 2_545 no
C37 H72 2.86(2) . 4_455 no
C38 H72 2.86(2) . 4_455 no
C43 H70' 2.81(2) . 2_555 no
C45 H64 2.97(2) . 4_454 no
C50 H70 2.90(2) . 1_455 no
C51 H70 2.87(2) . 1_455 no
C52 H65 2.98(2) . 3_556 no
C57 H72" 2.91(3) . 1_455 no
C62 H69' 3.047(19) . . no
C66 H72 3.09(2) . 2_545 no
C67 H69' 2.91(2) . . no
C71 H68 2.61(2) . . no
H63 C12 2.98(2) . . no
H63 C1 2.81(2) . . no
H63 C6 2.76(2) . . no
H64 C45 2.97(2) . 4_555 no
H65 C12 2.90(2) . 3_656 no
H65 C52 2.98(2) . 3_556 no
H66 C28 3.05(2) . 2_545 no
H66 O1 2.52(2) . 2_545 no
H67 C2 3.08(2) . . no
H67 H72' 2.56(4) . 2_545 no
H68 O1 2.70(2) . . no
H68 C9 2.56(2) . . no
H68 C10 2.63(2) . . no
H68 C11 2.81(2) . . no
H68 C12 2.91(2) . . no
H68 C71 2.61(2) . . no
H68' C12 3.00(2) . . no
H69 O1 2.69(2) . . no
H69 C2 2.89(2) . . no
H69 C12 2.71(2) . . no
H69 H76 2.48(3) . 4_454 no
H69' C27 3.09(2) . 2_545 no
H69' C26 3.09(2) . 2_545 no
H69' C62 3.047(19) . . no
H69' C67 2.91(2) . . no
H70 C51 2.87(2) . 1_655 no
H70 C50 2.90(2) . 1_655 no
H70' C43 2.81(2) . 2_545 no
H72 O1 2.50(2) . . no
H72 C66 3.09(2) . 2_555 no
H72 C37 2.86(2) . 4_554 no
H72 C38 2.86(2) . 4_554 no
H72' C11 2.71(3) . . no
H72' H67 2.56(4) . 2_555 no
H72' O1 2.75(3) . . no

H72" C57 2.91(3) . 1_655 no
H72" C16 3.07(3) . 2_555 no
H75 O1 2.75(2) . 4_555 no
H76 C25 3.06(2) . 3_666 no
H76 H69 2.48(3) . 4_555 no
H77 C8 2.90(2) . 3_666 no
H77 C24 2.62(2) . 3_666 no
H78 C13 2.75(2) . 2_555 no
H78 C14 3.02(2) . 2_555 no
H78 C30 2.78(2) . 2_555 no
H78 C31 3.08(2) . 2_555 no

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)

C66 H66 O1 1.00(2) 2.52(2) 3.409(3) 148.4(17) 2_545 yes
C72 H72' C11 1.07(3) 2.71(3) 3.649(3) 147(2) . yes

#####

data_c150h33c
_database_code_CSD 211977

#####

5. CHEMICAL DATA

_chemical_name_systematic
;
Methyl 5-(3'H-cyclopropa[1,9](C60-Ih)[5,6]fullerenyl)-5-phenylpentanoate.
;
_chemical_name_common
;Methyl 5-(3'H-cyclopropa(1,9)(C60-Ih)(5,6)fullerenyl)-5-phenylpentanoate.
;
_chemical_melting_point ?
_chemical_formula_moiety '2(C72 H14 O2), C6 H5 Cl'
_chemical_formula_structural ?
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum 'C150 H33 Cl O4'
_chemical_formula_weight 1934.21
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#####

6. CRYSTAL DATA

```
_symmetry_cell_setting      Triclinic
_symmetry_space_group_name_Hall '-P 1'
_symmetry_space_group_name_H-M 'P -1'
```

```
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,-y,-z
```

```
_cell_length_a      13.8333(9)
_cell_length_b      15.288(1)
_cell_length_c      19.249(1)
_cell_angle_alpha    80.259(1)
_cell_angle_beta     78.557(1)
_cell_angle_gamma    80.406(1)
_cell_volume         3894.9(4)
_cell_formula_units_Z 2
```

```
_cell_measurement_temperature 90
_cell_measurement_reflns_used  4343
_cell_measurement_theta_min    2.18
_cell_measurement_theta_max    26.52
_cell_special_details
```

```
;
The final unit cell was obtained from the xyz centroids of
4343 reflections after integration using the SAINT software
package (Bruker, 2000).
```

```
The intensity data were corrected for decay and absorption
using SADABS (Sheldrick, 2000).
;
```

```
_exptl_crystal_description  'triangle platelet'
_exptl_crystal_colour        reddish

_exptl_crystal_size_max     0.18
_exptl_crystal_size_mid     0.15
_exptl_crystal_size_min     0.10
_exptl_crystal_size_rad     ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffrn 1.648
_exptl_crystal_density_method 'Not Measured'
_exptl_crystal_F_000        1964
_exptl_absorpt_coefficient_mu 0.131
_exptl_absorpt_correction_type Semi-empirical
_exptl_absorpt_process_details 'SADABS (Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min 0.9768
_exptl_absorpt_correction_T_max 0.9870
```

```
#####
```

7. EXPERIMENTAL DATA

```
_exptl_special_details
; ?
;
_diffrn_ambient_temperature 90(2)
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type      MoK $\alpha$ 
_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-temperature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number        ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time ?

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number           34221
_diffrn_reflns_av_R_equivalents 0.0517
_diffrn_reflns_av_sigmaI/netI   0.0991
_diffrn_reflns_limit_h_min      -17
_diffrn_reflns_limit_h_max      17
_diffrn_reflns_limit_k_min      -19
_diffrn_reflns_limit_k_max      19
_diffrn_reflns_limit_l_min      -24
_diffrn_reflns_limit_l_max      21
_diffrn_reflns_theta_min        2.18
_diffrn_reflns_theta_max        26.37
_diffrn_measured_fraction_theta_max 0.987
_diffrn_reflns_theta_full       26.37
_diffrn_measured_fraction_theta_full 0.987

_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
_reflns_number_total            15737
_reflns_number_gt               9339
_reflns_threshold_expression      $I > 2\sigma(I)$ 

_computing_data_collection       'SMART, Bruker Version 5.168, 2000'
_computing_cell_refinement       'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction        'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
SIR-97 (Altomare et al., 1997)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2000)
PLATON (Spek, 1994)
;
_computing_publication_material 'PLATON (Spek, 1990)'

#=====

# 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 fullcycle
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0454P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_solution_primary patterson
_refine_ls_solution_secondary direct
_refine_ls_solution_hydrogens difmap
_refine_ls_hydrogen_treatment refall
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 15737
_refine_ls_number_parameters 1544
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.1080
_refine_ls_R_factor_gt 0.0532
_refine_ls_wR_factor_ref 0.1184
_refine_ls_wR_factor_gt 0.1009
_refine_ls_goodness_of_fit_ref 0.977
_refine_ls_restrained_S_all 0.977
_refine_ls_shift/su_max 0.340
_refine_ls_shift/su_mean 0.005

_refine_diff_density_max 0.279
_refine_diff_density_min -0.279
_refine_diff_density_rms 0.056

#=====

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Cl31 Cl Uani 0.03025(14) 0.30906(12) 0.06906(10) 0.500 0.0660(7) . .
C31 C Uani 0.0126(3) 0.4230(2) 0.0280(3) 0.500 0.029(2) . .
C32 C Uani 0.0916(3) 0.4723(3) 0.0144(3) 0.500 0.032(3) . .
C33 C Uani 0.0803(4) 0.5602(3) -0.0191(3) 0.500 0.042(3) . .
C34 C Uani -0.0101(4) 0.5989(3) -0.0389(3) 0.500 0.057(4) . .
C35 C Uani -0.0891(4) 0.5497(3) -0.0253(3) 0.500 0.051(3) . .
C36 C Uani -0.0777(4) 0.4617(3) 0.0082(3) 0.500 0.036(3) . .
H32 H Uiso 0.15346 0.44580 0.02803 0.500 0.0388 . .
H33 H Uiso 0.13439 0.59394 -0.02840 0.500 0.0502 . .
H34 H Uiso -0.01784 0.65913 -0.06183 0.500 0.0677 . .

```

H35 H Uiso -0.15096 0.57615 -0.03885 0.500 0.0615 . .
H36 H Uiso -0.13183 0.42797 0.01753 0.500 0.0428 . .
Cl41 Cl Uani 0.18808(10) 0.53356(9) 0.44696(8) 0.500 0.0339(5) . .
C41 C Uani 0.0662(2) 0.5176(2) 0.4808(2) 0.500 0.0237(17) . .
C42 C Uani -0.0006(3) 0.5200(2) 0.43535(18) 0.500 0.029(2) . .
C43 C Uani -0.0983(2) 0.5074(2) 0.4634(2) 0.500 0.039(2) . .
C44 C Uiso -0.12932 0.49251 0.53679 0.500(6) 0.0378(2) . .
C45 C Uani -0.0626(3) 0.4901(2) 0.58225(19) 0.500 0.034(2) . .
C46 C Uani 0.0352(3) 0.5027(2) 0.5543(2) 0.500 0.032(2) . .
H42 H Uiso 0.02061 0.53023 0.38497 0.500 0.0346 . .
H43 H Uiso -0.14414 0.50910 0.43220 0.500 0.0471 . .
H44 H Uiso -0.19637 0.48389 0.55600 0.500 0.0454 . .
H45 H Uiso -0.08384 0.47989 0.63264 0.500 0.0411 . .
H46 H Uiso 0.08097 0.50102 0.58542 0.500 0.0388 . .
O11 O Uani -0.06945(13) 0.54030(12) 0.28514(9) 1.000 0.0314(6) . .
O12 O Uani -0.03770(13) 0.52452(11) 0.16877(9) 1.000 0.0293(6) . .
C11 C Uani 0.38899(17) 0.37397(15) 0.23324(13) 1.000 0.0186(8) . .
C12 C Uani 0.40245(18) 0.26859(15) 0.22321(13) 1.000 0.0182(8) . .
C13 C Uani 0.50198(18) 0.23277(15) 0.18481(13) 1.000 0.0201(8) . .
C14 C Uani 0.57502(18) 0.28550(15) 0.15284(12) 1.000 0.0184(8) . .
C15 C Uani 0.56300(18) 0.38054(15) 0.16272(12) 1.000 0.0188(8) . .
C16 C Uani 0.47889(17) 0.41913(15) 0.20382(12) 1.000 0.0176(8) . .
C17 C Uani 0.48867(18) 0.47627(15) 0.25336(13) 1.000 0.0199(8) . .
C18 C Uani 0.41565(18) 0.45972(15) 0.31769(13) 1.000 0.0194(8) . .
C19 C Uani 0.36048(17) 0.39176(15) 0.30885(13) 1.000 0.0195(8) . .
C110 C Uani 0.33577(17) 0.32678(16) 0.36604(13) 1.000 0.0198(8) . .
C111 C Uani 0.34801(17) 0.23158(16) 0.35662(13) 1.000 0.0203(8) . .
C112 C Uani 0.38467(18) 0.20495(15) 0.29060(13) 1.000 0.0201(8) . .
C113 C Uani 0.45878(18) 0.12706(15) 0.28462(13) 1.000 0.0198(8) . .
C114 C Uani 0.53039(18) 0.14378(15) 0.22010(13) 1.000 0.0201(8) . .
C115 C Uani 0.62977(18) 0.10786(16) 0.21822(13) 1.000 0.0221(8) . .
C116 C Uani 0.70615(18) 0.16250(16) 0.18365(13) 1.000 0.0219(8) . .
C117 C Uani 0.67899(18) 0.25004(16) 0.15251(12) 1.000 0.0211(8) . .
C118 C Uani 0.73123(18) 0.32080(16) 0.16072(12) 1.000 0.0218(8) . .
C119 C Uani 0.65993(18) 0.40089(16) 0.16764(13) 1.000 0.0210(8) . .
C120 C Uani 0.66805(18) 0.45964(16) 0.21371(14) 1.000 0.0231(8) . .
C121 C Uani 0.58062(19) 0.49760(15) 0.25769(13) 1.000 0.0212(8) . .
C122 C Uani 0.60490(19) 0.50285(15) 0.32665(14) 1.000 0.0242(9) . .
C123 C Uani 0.5356(2) 0.48617(15) 0.38813(14) 1.000 0.0243(9) . .
C124 C Uani 0.43868(19) 0.46451(15) 0.38419(14) 1.000 0.0233(8) . .
C125 C Uani 0.41084(19) 0.39777(16) 0.44420(13) 1.000 0.0244(8) . .
C126 C Uani 0.36080(18) 0.33000(16) 0.43523(13) 1.000 0.0226(8) . .
C127 C Uani 0.38837(18) 0.23899(17) 0.46785(13) 1.000 0.0239(8) . .
C128 C Uani 0.38000(18) 0.17877(16) 0.42011(13) 1.000 0.0219(8) . .
C129 C Uani 0.44797(18) 0.10140(15) 0.41402(13) 1.000 0.0223(8) . .
C130 C Uani 0.48881(18) 0.07512(15) 0.34499(13) 1.000 0.0211(8) . .
C131 C Uani 0.59252(19) 0.03788(15) 0.34349(14) 1.000 0.0225(9) . .
C132 C Uani 0.66158(19) 0.05409(15) 0.28162(13) 1.000 0.0226(8) . .
C133 C Uani 0.75822(18) 0.07601(16) 0.28558(14) 1.000 0.0233(8) . .
C134 C Uani 0.78542(18) 0.14299(16) 0.22495(13) 1.000 0.0240(8) . .
C135 C Uani 0.83555(17) 0.21088(17) 0.23313(13) 1.000 0.0243(8) . .
C136 C Uani 0.80794(18) 0.30162(17) 0.20043(13) 1.000 0.0240(8) . .
C137 C Uani 0.81594(18) 0.36220(17) 0.24886(14) 1.000 0.0251(9) . .
C138 C Uani 0.74749(19) 0.43941(16) 0.25544(14) 1.000 0.0253(9) . .
C139 C Uani 0.70844(19) 0.46614(16) 0.32519(14) 1.000 0.0254(9) . .
C140 C Uani 0.73939(19) 0.41484(16) 0.38561(14) 1.000 0.0253(9) . .
C141 C Uani 0.6671(2) 0.39753(16) 0.45013(14) 1.000 0.0257(9) . .
C142 C Uani 0.5674(2) 0.43229(16) 0.45160(13) 1.000 0.0248(9) . .
C143 C Uani 0.4898(2) 0.37786(16) 0.48614(13) 1.000 0.0255(8) . .
C144 C Uani 0.51661(19) 0.29067(17) 0.51760(12) 1.000 0.0244(8) . .
C145 C Uani 0.46377(19) 0.22019(16) 0.50882(13) 1.000 0.0236(8) . .
C146 C Uani 0.53535(19) 0.13953(16) 0.50255(13) 1.000 0.0229(8) . .
C147 C Uani 0.52774(18) 0.08195(15) 0.45604(13) 1.000 0.0221(8) . .
C148 C Uani 0.61678(19) 0.04224(15) 0.41259(13) 1.000 0.0220(8) . .
C149 C Uani 0.70922(19) 0.06318(15) 0.41685(13) 1.000 0.0228(8) . .
C150 C Uani 0.78148(18) 0.08013(15) 0.35203(13) 1.000 0.0223(8) . .
C151 C Uani 0.83413(18) 0.15094(16) 0.36049(13) 1.000 0.0223(8) . .

C152	C	Uani	0.86032(17)	0.21521(17)	0.30238(14)	1.000	0.0240(8)	. .
C153	C	Uani	0.84810(18)	0.30861(17)	0.31220(14)	1.000	0.0254(9)	. .
C154	C	Uani	0.81070(18)	0.33476(17)	0.37872(14)	1.000	0.0256(9)	. .
C155	C	Uani	0.78259(19)	0.26751(17)	0.43975(13)	1.000	0.0238(9)	. .
C156	C	Uani	0.79472(18)	0.17752(16)	0.43072(13)	1.000	0.0215(8)	. .
C157	C	Uani	0.71755(18)	0.12350(15)	0.46531(13)	1.000	0.0210(8)	. .
C158	C	Uani	0.63202(19)	0.16088(16)	0.50681(12)	1.000	0.0216(8)	. .
C159	C	Uani	0.61981(19)	0.25444(17)	0.51636(13)	1.000	0.0244(9)	. .
C160	C	Uani	0.6937(2)	0.30656(16)	0.48361(13)	1.000	0.0241(8)	. .
C161	C	Uani	0.32667(18)	0.33907(15)	0.19135(13)	1.000	0.0195(8)	. .
C162	C	Uani	0.34298(17)	0.36102(15)	0.11100(13)	1.000	0.0198(8)	. .
C163	C	Uani	0.33142(19)	0.29660(17)	0.07118(14)	1.000	0.0230(8)	. .
C164	C	Uani	0.33906(19)	0.31543(17)	-0.00226(14)	1.000	0.0266(9)	. .
C165	C	Uani	0.36056(19)	0.39861(17)	-0.03763(14)	1.000	0.0262(9)	. .
C166	C	Uani	0.37235(19)	0.46310(17)	0.00123(14)	1.000	0.0256(9)	. .
C167	C	Uani	0.36291(18)	0.44475(16)	0.07529(14)	1.000	0.0221(8)	. .
C168	C	Uani	0.21763(19)	0.33415(17)	0.22466(15)	1.000	0.0223(8)	. .
C169	C	Uani	0.15245(19)	0.42508(17)	0.21640(15)	1.000	0.0229(8)	. .
C170	C	Uani	0.0438(2)	0.41329(18)	0.24489(17)	1.000	0.0295(9)	. .
C171	C	Uani	-0.02695(18)	0.49910(17)	0.23678(14)	1.000	0.0233(9)	. .
C172	C	Uani	-0.1092(2)	0.60340(19)	0.15503(17)	1.000	0.0310(10)	. .
H163	H	Uiso	0.31701	0.23793	0.09397	1.00(3)	0.0232(16)	. .
H164	H	Uiso	0.33184	0.26880	-0.02999	1.00(4)	0.0280(17)	. .
H165	H	Uiso	0.36295	0.41323	-0.09044	1.00(3)	0.0169(16)	. .
H166	H	Uiso	0.38837	0.52291	-0.02426	1.00(3)	0.0300(17)	. .
H167	H	Uiso	0.37090	0.49306	0.10292	1.00(3)	0.0247(16)	. .
H168	H	Uiso	0.21331	0.31267	0.27515	1.00(3)	0.0289(17)	. .
H168'	H	Uiso	0.18943	0.29509	0.19976	1.00(4)	0.0246(17)	. .
H169	H	Uiso	0.17473	0.46564	0.24416	1.00(4)	0.0226(16)	. .
H169'	H	Uiso	0.15710	0.45225	0.16444	1.00(3)	0.0284(17)	. .
H170	H	Uiso	0.02619	0.36738	0.21612	1.00(4)	0.048(2)	. .
H170'	H	Uiso	0.03803	0.39044	0.29659	1.00(4)	0.0463(19)	. .
H172	H	Uiso	-0.10189	0.65552	0.18418	1.00(5)	0.062(2)	. .
H172'	H	Uiso	-0.09360	0.62155	0.09795	1.00(5)	0.090(2)	. .
H172"	H	Uiso	-0.17858	0.59100	0.17574	1.00(5)	0.072(2)	. .
O21	O	Uani	-0.31589(15)	0.70087(13)	0.21471(11)	1.000	0.0442(8)	. .
O22	O	Uani	-0.28656(16)	0.83984(14)	0.21476(11)	1.000	0.0481(8)	. .
C21	C	Uani	0.00301(18)	0.79062(15)	0.31163(13)	1.000	0.0193(8)	. .
C22	C	Uani	-0.01259(18)	0.89795(15)	0.31377(13)	1.000	0.0189(8)	. .
C23	C	Uani	0.07022(18)	0.93114(15)	0.33542(12)	1.000	0.0187(8)	. .
C24	C	Uani	0.14935(18)	0.87591(16)	0.36022(12)	1.000	0.0202(8)	. .
C25	C	Uani	0.16353(18)	0.77881(16)	0.35806(12)	1.000	0.0201(8)	. .
C26	C	Uani	0.09770(18)	0.74087(15)	0.33123(12)	1.000	0.0193(8)	. .
C27	C	Uani	0.13564(18)	0.67550(15)	0.28285(13)	1.000	0.0197(8)	. .
C28	C	Uani	0.07511(18)	0.69044(15)	0.22775(13)	1.000	0.0197(8)	. .
C29	C	Uani	-0.00125(17)	0.76535(15)	0.24103(13)	1.000	0.0189(8)	. .
C210	C	Uani	-0.02706(17)	0.82539(15)	0.18359(13)	1.000	0.0187(8)	. .
C211	C	Uani	-0.04109(17)	0.92282(15)	0.18561(13)	1.000	0.0189(8)	. .
C212	C	Uani	-0.02822(17)	0.95546(15)	0.24532(13)	1.000	0.0189(8)	. .
C213	C	Uani	0.02698(17)	1.03007(15)	0.23592(13)	1.000	0.0200(8)	. .
C214	C	Uani	0.08710(18)	1.01517(15)	0.29085(13)	1.000	0.0204(8)	. .
C215	C	Uani	0.17994(19)	1.04434(16)	0.27655(13)	1.000	0.0226(8)	. .
C216	C	Uani	0.26234(19)	0.98676(16)	0.30363(13)	1.000	0.0222(8)	. .
C217	C	Uani	0.24711(18)	0.90434(17)	0.34365(13)	1.000	0.0219(8)	. .
C218	C	Uani	0.32089(19)	0.82697(16)	0.33168(13)	1.000	0.0228(8)	. .
C219	C	Uani	0.26966(18)	0.74981(16)	0.33971(13)	1.000	0.0213(8)	. .
C220	C	Uani	0.30583(18)	0.68378(15)	0.29666(13)	1.000	0.0216(8)	. .
C221	C	Uani	0.23717(18)	0.64556(15)	0.26673(13)	1.000	0.0211(8)	. .
C222	C	Uani	0.28138(18)	0.63017(15)	0.19474(14)	1.000	0.0219(8)	. .
C223	C	Uani	0.22402(18)	0.64432(15)	0.14141(14)	1.000	0.0223(8)	. .
C224	C	Uani	0.11813(18)	0.67497(15)	0.15841(13)	1.000	0.0213(8)	. .
C225	C	Uani	0.08879(18)	0.73663(16)	0.09857(13)	1.000	0.0209(8)	. .
C226	C	Uani	0.01834(17)	0.81095(16)	0.11122(13)	1.000	0.0187(8)	. .
C227	C	Uani	0.03276(18)	0.89738(16)	0.06899(13)	1.000	0.0202(8)	. .
C228	C	Uani	-0.00363(17)	0.96536(16)	0.11521(13)	1.000	0.0213(8)	. .
C229	C	Uani	0.04573(17)	1.04031(15)	0.10616(13)	1.000	0.0203(8)	. .
C230	C	Uani	0.06127(18)	1.07361(15)	0.16809(13)	1.000	0.0198(8)	. .

C231	C	Uani	0.15849(18)	1.10313(15)	0.15230(13)	1.000	0.0207(8)	.	.
C232	C	Uani	0.21682(18)	1.08860(15)	0.20565(13)	1.000	0.0213(8)	.	.
C233	C	Uani	0.32246(18)	1.05812(15)	0.18845(13)	1.000	0.0208(8)	.	.
C234	C	Uani	0.35038(18)	0.99516(16)	0.24912(13)	1.000	0.0212(8)	.	.
C235	C	Uani	0.42113(18)	0.92132(16)	0.23785(13)	1.000	0.0222(8)	.	.
C236	C	Uani	0.40666(18)	0.83477(16)	0.28001(13)	1.000	0.0222(8)	.	.
C237	C	Uani	0.44322(18)	0.76649(16)	0.23411(14)	1.000	0.0237(8)	.	.
C238	C	Uani	0.39391(17)	0.69226(15)	0.24198(13)	1.000	0.0213(8)	.	.
C239	C	Uani	0.37864(18)	0.65923(15)	0.17925(14)	1.000	0.0242(8)	.	.
C240	C	Uani	0.41415(18)	0.70126(16)	0.11093(14)	1.000	0.0233(8)	.	.
C241	C	Uani	0.35385(18)	0.71579(16)	0.05568(14)	1.000	0.0242(8)	.	.
C242	C	Uani	0.26036(19)	0.68794(16)	0.07023(13)	1.000	0.0221(8)	.	.
C243	C	Uani	0.17707(19)	0.74532(16)	0.04393(13)	1.000	0.0229(8)	.	.
C244	C	Uani	0.19045(18)	0.82792(17)	0.00400(12)	1.000	0.0220(8)	.	.
C245	C	Uani	0.11691(18)	0.90534(16)	0.01644(13)	1.000	0.0220(8)	.	.
C246	C	Uani	0.16854(18)	0.98263(16)	0.00774(13)	1.000	0.0226(8)	.	.
C247	C	Uani	0.13402(18)	1.04865(15)	0.05133(13)	1.000	0.0211(8)	.	.
C248	C	Uani	0.20335(18)	1.08777(15)	0.08032(13)	1.000	0.0218(8)	.	.
C249	C	Uani	0.30518(18)	1.05865(15)	0.06360(13)	1.000	0.0206(8)	.	.
C250	C	Uani	0.36604(18)	1.04371(15)	0.11914(13)	1.000	0.0214(8)	.	.
C251	C	Uani	0.43937(17)	0.96611(15)	0.10734(13)	1.000	0.0207(8)	.	.
C252	C	Uani	0.46640(17)	0.90625(16)	0.16576(14)	1.000	0.0223(8)	.	.
C253	C	Uani	0.47972(17)	0.81028(16)	0.16328(14)	1.000	0.0238(8)	.	.
C254	C	Uani	0.46565(17)	0.77843(16)	0.10321(14)	1.000	0.0233(8)	.	.
C255	C	Uani	0.43727(18)	0.84105(16)	0.04267(13)	1.000	0.0225(8)	.	.
C256	C	Uani	0.42428(18)	0.93248(16)	0.04463(13)	1.000	0.0222(8)	.	.
C257	C	Uani	0.34148(18)	0.98984(16)	0.01792(13)	1.000	0.0222(8)	.	.
C258	C	Uani	0.27405(19)	0.95297(16)	-0.00927(12)	1.000	0.0223(8)	.	.
C259	C	Uani	0.28817(19)	0.85736(17)	-0.01205(13)	1.000	0.0244(9)	.	.
C260	C	Uani	0.36760(18)	0.80271(16)	0.01333(13)	1.000	0.0230(8)	.	.
C261	C	Uani	-0.08286(18)	0.83616(15)	0.36084(13)	1.000	0.0201(8)	.	.
C262	C	Uani	-0.07994(18)	0.82421(16)	0.43985(13)	1.000	0.0220(8)	.	.
C263	C	Uani	-0.0696(2)	0.74017(18)	0.48030(14)	1.000	0.0285(9)	.	.
C264	C	Uani	-0.0722(2)	0.73236(19)	0.55345(15)	1.000	0.0355(10)	.	.
C265	C	Uani	-0.0833(2)	0.80724(19)	0.58634(15)	1.000	0.0326(10)	.	.
C266	C	Uani	-0.0932(2)	0.89159(19)	0.54651(15)	1.000	0.0313(10)	.	.
C267	C	Uani	-0.09206(19)	0.89978(17)	0.47363(14)	1.000	0.0258(9)	.	.
C268	C	Uani	-0.18618(19)	0.84078(16)	0.34212(15)	1.000	0.0233(8)	.	.
C269	C	Uani	-0.2218(2)	0.74896(17)	0.35360(15)	1.000	0.0249(8)	.	.
C270	C	Uani	-0.3207(2)	0.75252(19)	0.32677(14)	1.000	0.0258(9)	.	.
C271	C	Uani	-0.30842(19)	0.75956(19)	0.24708(15)	1.000	0.0295(9)	.	.
C272	C	Uani	-0.2638(3)	0.8501(3)	0.13676(18)	1.000	0.0646(14)	.	.
H263	H	Uiso	-0.06359	0.68799	0.45711	1.00(3)	0.0254(16)	.	.
H264	H	Uiso	-0.06455	0.67561	0.58111	1.00(4)	0.0327(18)	.	.
H265	H	Uiso	-0.08292	0.80469	0.63621	1.00(3)	0.0279(17)	.	.
H266	H	Uiso	-0.09944	0.94586	0.56869	1.00(4)	0.0400(18)	.	.
H267	H	Uiso	-0.09439	0.96116	0.44495	1.00(3)	0.0294(17)	.	.
H268	H	Uiso	-0.23547	0.88214	0.37512	1.00(3)	0.0240(17)	.	.
H268'	H	Uiso	-0.18655	0.87075	0.29074	1.00(3)	0.0225(16)	.	.
H269	H	Uiso	-0.22863	0.72578	0.40698	1.00(3)	0.0309(17)	.	.
H269'	H	Uiso	-0.16746	0.70222	0.32774	1.00(4)	0.055(2)	.	.
H270	H	Uiso	-0.36996	0.80660	0.34140	1.00(3)	0.0299(18)	.	.
H270'	H	Uiso	-0.34413	0.69461	0.34572	1.00(4)	0.0351(18)	.	.
H272	H	Uiso	-0.32454	0.84719	0.11987	1.00(5)	0.060(2)	.	.
H272'	H	Uiso	-0.24401	0.91235	0.12077	1.00(6)	0.101(3)	.	.
H272"	H	Uiso	-0.20599	0.80219	0.11951	1.00(6)	0.139(3)	.	.

loop_

_atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12

O11	0.0325(11)	0.0352(11)	0.0262(11)	-0.0065(9)	-0.0028(9)	-0.0048(9)
O12	0.0304(11)	0.0294(10)	0.0263(11)	-0.0028(8)	-0.0050(9)	0.0000(8)

C11 0.0178(14) 0.0162(12) 0.0208(14) -0.0008(10) -0.0032(11) -0.0014(10)
C12 0.0215(14) 0.0171(12) 0.0181(14) -0.0018(10) -0.0067(11) -0.0057(10)
C13 0.0259(15) 0.0220(13) 0.0152(14) -0.0051(11) -0.0099(12) -0.0009(11)
C14 0.0230(14) 0.0226(13) 0.0107(13) -0.0029(10) -0.0059(11) -0.0022(11)
C15 0.0216(14) 0.0206(13) 0.0132(13) 0.0035(10) -0.0055(11) -0.0035(11)
C16 0.0197(14) 0.0157(12) 0.0178(14) 0.0041(10) -0.0090(11) -0.0034(10)
C17 0.0243(14) 0.0122(12) 0.0215(14) 0.0019(10) -0.0068(12) 0.0012(10)
C18 0.0203(14) 0.0145(12) 0.0219(14) -0.0049(10) -0.0046(11) 0.0054(10)
C19 0.0172(13) 0.0178(13) 0.0216(14) -0.0024(11) -0.0031(11) 0.0022(10)
C110 0.0132(13) 0.0240(14) 0.0203(14) -0.0008(11) -0.0004(11) -0.0025(10)
C111 0.0146(13) 0.0236(14) 0.0222(15) 0.0029(11) -0.0027(11) -0.0079(11)
C112 0.0217(14) 0.0181(13) 0.0237(15) -0.0005(11) -0.0081(12) -0.0091(11)
C113 0.0232(14) 0.0154(12) 0.0249(15) -0.0044(11) -0.0089(12) -0.0075(11)
C114 0.0257(15) 0.0175(13) 0.0209(14) -0.0076(11) -0.0096(12) -0.0024(11)
C115 0.0269(15) 0.0207(13) 0.0218(15) -0.0143(11) -0.0066(12) 0.0022(11)
C116 0.0252(15) 0.0240(14) 0.0159(14) -0.0099(11) -0.0012(11) 0.0026(11)
C117 0.0212(14) 0.0293(14) 0.0106(13) -0.0029(11) -0.0003(11) 0.0002(11)
C118 0.0219(14) 0.0277(14) 0.0121(13) 0.0012(11) 0.0027(11) -0.0034(11)
C119 0.0183(14) 0.0236(14) 0.0187(14) 0.0074(11) -0.0025(11) -0.0074(11)
C120 0.0232(15) 0.0194(13) 0.0261(15) 0.0075(11) -0.0058(12) -0.0107(11)
C121 0.0288(15) 0.0108(12) 0.0249(15) 0.0053(11) -0.0098(12) -0.0070(11)
C122 0.0333(16) 0.0117(12) 0.0313(16) -0.0035(11) -0.0116(13) -0.0057(11)
C123 0.0380(17) 0.0123(12) 0.0258(16) -0.0084(11) -0.0091(13) -0.0024(12)
C124 0.0270(15) 0.0144(13) 0.0264(15) -0.0069(11) -0.0026(12) 0.0043(11)
C125 0.0297(16) 0.0240(14) 0.0177(14) -0.0088(11) -0.0006(12) 0.0027(12)
C126 0.0200(14) 0.0272(14) 0.0163(14) -0.0054(11) 0.0033(11) 0.0034(11)
C127 0.0199(14) 0.0299(15) 0.0176(14) 0.0005(11) 0.0051(11) -0.0055(11)
C128 0.0172(14) 0.0262(14) 0.0206(14) 0.0040(11) 0.0009(11) -0.0105(11)
C129 0.0252(15) 0.0153(13) 0.0257(15) 0.0074(11) -0.0061(12) -0.0097(11)
C130 0.0271(15) 0.0127(12) 0.0262(15) 0.0011(11) -0.0084(12) -0.0096(11)
C131 0.0306(16) 0.0086(12) 0.0291(16) -0.0004(11) -0.0097(13) -0.0015(11)
C132 0.0306(16) 0.0138(12) 0.0253(15) -0.0068(11) -0.0094(12) 0.0014(11)
C133 0.0248(15) 0.0184(13) 0.0249(15) -0.0049(11) -0.0054(12) 0.0051(11)
C134 0.0186(14) 0.0276(14) 0.0228(15) -0.0063(12) -0.0006(12) 0.0041(11)
C135 0.0118(13) 0.0358(16) 0.0218(15) -0.0027(12) 0.0003(11) 0.0013(11)
C136 0.0158(14) 0.0331(15) 0.0193(14) 0.0015(12) 0.0015(11) -0.0036(12)
C137 0.0160(14) 0.0341(15) 0.0254(16) 0.0045(12) -0.0051(12) -0.0113(12)
C138 0.0237(15) 0.0254(14) 0.0282(16) 0.0077(12) -0.0055(12) -0.0175(12)
C139 0.0310(16) 0.0171(13) 0.0331(17) -0.0009(12) -0.0124(13) -0.0118(12)
C140 0.0294(16) 0.0227(14) 0.0307(16) -0.0064(12) -0.0127(13) -0.0116(12)
C141 0.0355(17) 0.0252(14) 0.0227(15) -0.0083(12) -0.0124(13) -0.0084(12)
C142 0.0353(16) 0.0225(14) 0.0218(15) -0.0127(12) -0.0101(13) -0.0032(12)
C143 0.0342(16) 0.0250(14) 0.0180(14) -0.0106(11) -0.0041(12) 0.0011(12)
C144 0.0331(16) 0.0302(15) 0.0097(13) -0.0063(11) -0.0014(12) -0.0030(12)
C145 0.0284(15) 0.0284(14) 0.0107(13) 0.0021(11) 0.0008(12) -0.0041(12)
C146 0.0259(15) 0.0237(14) 0.0160(14) 0.0060(11) -0.0014(12) -0.0065(12)
C147 0.0269(15) 0.0176(13) 0.0205(14) 0.0086(11) -0.0043(12) -0.0107(11)
C148 0.0297(15) 0.0133(12) 0.0228(15) 0.0040(11) -0.0089(12) -0.0039(11)
C149 0.0286(15) 0.0153(13) 0.0229(15) 0.0019(11) -0.0093(12) 0.0026(11)
C150 0.0203(14) 0.0187(13) 0.0269(16) -0.0023(11) -0.0089(12) 0.0047(11)
C151 0.0180(14) 0.0245(14) 0.0236(15) -0.0011(12) -0.0081(12) 0.0027(11)
C152 0.0109(13) 0.0323(15) 0.0277(16) -0.0003(12) -0.0052(12) -0.0018(11)
C153 0.0147(14) 0.0309(15) 0.0323(17) 0.0027(12) -0.0086(12) -0.0100(11)
C154 0.0228(15) 0.0301(15) 0.0286(16) -0.0005(12) -0.0117(12) -0.0118(12)
C155 0.0248(15) 0.0295(15) 0.0222(15) 0.0003(12) -0.0155(12) -0.0083(12)
C156 0.0206(14) 0.0253(14) 0.0206(14) 0.0005(11) -0.0121(12) -0.0021(11)
C157 0.0253(15) 0.0203(13) 0.0177(14) 0.0024(11) -0.0098(12) -0.0022(11)
C158 0.0310(16) 0.0229(14) 0.0108(13) 0.0046(11) -0.0083(12) -0.0052(12)
C159 0.0335(16) 0.0291(15) 0.0119(14) -0.0019(11) -0.0092(12) -0.0031(12)
C160 0.0359(16) 0.0258(14) 0.0163(14) -0.0055(11) -0.0136(12) -0.0070(12)
C161 0.0185(14) 0.0182(13) 0.0229(14) 0.0004(11) -0.0067(11) -0.0051(10)
C162 0.0152(13) 0.0205(13) 0.0236(15) -0.0044(11) -0.0055(11) 0.0020(10)
C163 0.0226(15) 0.0202(14) 0.0256(15) 0.0005(12) -0.0065(12) -0.0020(11)
C164 0.0260(15) 0.0266(15) 0.0273(16) -0.0071(12) -0.0077(12) 0.0033(12)
C165 0.0278(16) 0.0309(15) 0.0156(14) 0.0017(12) -0.0046(12) 0.0038(12)
C166 0.0272(15) 0.0232(14) 0.0236(16) 0.0038(12) -0.0052(12) -0.0020(12)
C167 0.0206(14) 0.0222(14) 0.0236(15) -0.0045(12) -0.0064(12) 0.0011(11)

C168 0.0203(14) 0.0222(13) 0.0254(16) 0.0009(12) -0.0081(12) -0.0054(11)
C169 0.0199(14) 0.0256(14) 0.0231(15) 0.0004(12) -0.0029(12) -0.0077(11)
C170 0.0194(15) 0.0300(15) 0.0347(18) 0.0029(13) -0.0016(13) -0.0018(12)
C171 0.0189(14) 0.0283(15) 0.0245(16) 0.0008(12) -0.0030(12) -0.0135(12)
C172 0.0291(17) 0.0300(16) 0.0330(18) -0.0024(13) -0.0102(14) 0.0025(13)
O21 0.0448(13) 0.0497(13) 0.0397(13) -0.0169(11) -0.0121(10) 0.0057(10)
O22 0.0570(15) 0.0604(14) 0.0327(12) 0.0147(11) -0.0178(11) -0.0343(12)
C21 0.0208(14) 0.0192(13) 0.0176(14) -0.0018(11) -0.0008(11) -0.0055(11)
C22 0.0214(14) 0.0176(13) 0.0166(14) -0.0048(10) -0.0025(11) 0.0019(10)
C23 0.0236(14) 0.0193(13) 0.0125(13) -0.0082(10) 0.0022(11) -0.0016(11)
C24 0.0254(15) 0.0267(14) 0.0090(13) -0.0051(10) 0.0003(11) -0.0061(11)
C25 0.0261(15) 0.0222(13) 0.0115(13) 0.0022(10) -0.0046(11) -0.0047(11)
C26 0.0240(14) 0.0168(12) 0.0154(14) 0.0025(10) -0.0017(11) -0.0050(11)
C27 0.0217(14) 0.0154(12) 0.0213(14) 0.0030(10) -0.0033(11) -0.0072(11)
C28 0.0231(14) 0.0136(12) 0.0235(15) 0.0001(11) -0.0040(12) -0.0087(11)
C29 0.0140(13) 0.0199(13) 0.0230(15) -0.0006(11) -0.0017(11) -0.0076(10)
C210 0.0143(13) 0.0235(14) 0.0196(14) -0.0015(11) -0.0040(11) -0.0063(11)
C211 0.0140(13) 0.0228(13) 0.0192(14) -0.0010(11) -0.0053(11) 0.0002(10)
C212 0.0126(13) 0.0170(13) 0.0246(15) -0.0021(11) -0.0015(11) 0.0024(10)
C213 0.0182(14) 0.0166(13) 0.0225(14) -0.0056(11) -0.0006(11) 0.0048(10)
C214 0.0252(14) 0.0170(13) 0.0197(14) -0.0080(11) -0.0025(12) -0.0011(11)
C215 0.0312(16) 0.0184(13) 0.0221(15) -0.0111(11) -0.0044(12) -0.0061(12)
C216 0.0279(15) 0.0223(14) 0.0216(15) -0.0090(11) -0.0081(12) -0.0079(12)
C217 0.0256(15) 0.0311(15) 0.0127(14) -0.0039(11) -0.0084(11) -0.0072(12)
C218 0.0256(15) 0.0302(15) 0.0163(14) -0.0013(11) -0.0129(12) -0.0055(12)
C219 0.0245(14) 0.0213(13) 0.0169(14) 0.0064(11) -0.0098(12) -0.0014(11)
C220 0.0204(14) 0.0198(13) 0.0224(15) 0.0065(11) -0.0082(12) -0.0012(11)
C221 0.0238(15) 0.0117(12) 0.0248(15) 0.0040(11) -0.0041(12) -0.0009(11)
C222 0.0245(15) 0.0126(12) 0.0272(15) -0.0024(11) -0.0027(12) -0.0012(11)
C223 0.0246(15) 0.0147(12) 0.0288(16) -0.0109(11) 0.0007(12) -0.0047(11)
C224 0.0264(15) 0.0165(13) 0.0240(15) -0.0062(11) -0.0035(12) -0.0092(11)
C225 0.0225(14) 0.0261(14) 0.0206(14) -0.0101(11) -0.0058(12) -0.0123(11)
C226 0.0180(14) 0.0256(14) 0.0164(14) -0.0054(11) -0.0054(11) -0.0084(11)
C227 0.0194(14) 0.0251(14) 0.0191(14) 0.0004(11) -0.0113(11) -0.0053(11)
C228 0.0150(13) 0.0260(14) 0.0228(15) 0.0009(11) -0.0087(11) -0.0003(11)
C229 0.0186(14) 0.0199(13) 0.0202(14) 0.0030(11) -0.0075(11) 0.0023(11)
C230 0.0214(14) 0.0123(12) 0.0227(15) 0.0005(10) -0.0031(11) 0.0019(10)
C231 0.0271(15) 0.0102(12) 0.0234(15) 0.0020(10) -0.0044(12) -0.0033(10)
C232 0.0272(15) 0.0132(12) 0.0261(15) -0.0072(11) -0.0055(12) -0.0049(11)
C233 0.0237(14) 0.0161(13) 0.0257(15) -0.0036(11) -0.0065(12) -0.0083(11)
C234 0.0201(14) 0.0242(14) 0.0248(15) -0.0080(11) -0.0074(12) -0.0099(11)
C235 0.0179(14) 0.0256(14) 0.0272(16) -0.0047(12) -0.0103(12) -0.0064(11)
C236 0.0193(14) 0.0265(14) 0.0235(15) 0.0002(12) -0.0137(12) -0.0023(11)
C237 0.0167(14) 0.0262(14) 0.0269(16) 0.0036(12) -0.0110(12) 0.0020(11)
C238 0.0167(14) 0.0179(13) 0.0255(15) 0.0015(11) -0.0047(12) 0.0050(11)
C239 0.0213(14) 0.0154(13) 0.0320(16) -0.0052(12) -0.0018(12) 0.0066(11)
C240 0.0190(14) 0.0189(13) 0.0300(16) -0.0096(12) 0.0010(12) 0.0031(11)
C241 0.0236(15) 0.0235(14) 0.0250(15) -0.0115(12) 0.0032(12) -0.0025(12)
C242 0.0263(15) 0.0209(13) 0.0210(15) -0.0117(11) -0.0002(12) -0.0041(11)
C243 0.0276(15) 0.0275(14) 0.0190(14) -0.0121(12) -0.0050(12) -0.0087(12)
C244 0.0265(15) 0.0343(15) 0.0085(13) -0.0061(11) -0.0034(11) -0.0104(12)
C245 0.0269(15) 0.0308(15) 0.0122(14) 0.0004(11) -0.0098(12) -0.0109(12)
C246 0.0245(15) 0.0275(14) 0.0159(14) 0.0051(11) -0.0083(12) -0.0065(12)
C247 0.0238(14) 0.0193(13) 0.0183(14) 0.0069(11) -0.0087(12) -0.0011(11)
C248 0.0249(15) 0.0151(12) 0.0240(15) 0.0039(11) -0.0056(12) -0.0038(11)
C249 0.0260(15) 0.0163(13) 0.0190(14) 0.0051(11) -0.0025(12) -0.0107(11)
C250 0.0237(15) 0.0165(13) 0.0262(15) 0.0015(11) -0.0046(12) -0.0129(11)
C251 0.0160(14) 0.0209(13) 0.0251(15) -0.0004(11) -0.0009(11) -0.0088(11)
C252 0.0128(13) 0.0279(14) 0.0279(16) -0.0029(12) -0.0042(12) -0.0075(11)
C253 0.0120(13) 0.0249(14) 0.0330(16) 0.0001(12) -0.0051(12) -0.0013(11)
C254 0.0128(13) 0.0256(14) 0.0280(16) -0.0040(12) 0.0019(12) 0.0012(11)
C255 0.0162(14) 0.0274(14) 0.0199(14) -0.0022(11) 0.0056(11) -0.0034(11)
C256 0.0180(14) 0.0271(14) 0.0190(14) 0.0002(11) 0.0039(11) -0.0079(11)
C257 0.0236(15) 0.0242(14) 0.0163(14) 0.0033(11) 0.0022(11) -0.0093(11)
C258 0.0277(15) 0.0303(14) 0.0067(13) 0.0019(11) 0.0010(11) -0.0067(12)
C259 0.0284(16) 0.0344(15) 0.0107(14) -0.0072(11) 0.0016(12) -0.0074(12)
C260 0.0235(15) 0.0240(14) 0.0209(15) -0.0099(11) 0.0043(12) -0.0047(11)

```

C261 0.0213(14) 0.0186(13) 0.0184(14) -0.0023(11) 0.0011(11) -0.0029(11)
C262 0.0181(14) 0.0284(14) 0.0174(14) -0.0038(11) 0.0025(11) -0.0037(11)
C263 0.0370(17) 0.0251(15) 0.0233(16) -0.0036(12) -0.0005(13) -0.0094(12)
C264 0.050(2) 0.0283(16) 0.0246(17) 0.0068(13) -0.0047(14) -0.0080(14)
C265 0.0385(18) 0.0435(18) 0.0162(15) -0.0044(13) -0.0028(13) -0.0089(14)
C266 0.0334(17) 0.0356(17) 0.0243(16) -0.0087(13) -0.0004(13) -0.0043(13)
C267 0.0307(16) 0.0232(14) 0.0202(15) -0.0012(12) -0.0020(12) 0.0008(12)
C268 0.0208(14) 0.0220(14) 0.0245(15) -0.0022(12) -0.0014(12) -0.0001(11)
C269 0.0237(15) 0.0267(14) 0.0232(15) 0.0000(12) -0.0029(12) -0.0052(12)
C270 0.0221(15) 0.0292(15) 0.0257(16) -0.0013(12) -0.0024(12) -0.0073(12)
C271 0.0174(15) 0.0402(17) 0.0313(17) -0.0067(14) -0.0025(12) -0.0058(12)
C272 0.047(2) 0.119(3) 0.028(2) 0.034(2) -0.0193(17) -0.042(2)
Cl31 0.0674(13) 0.0598(12) 0.0579(12) -0.0035(10) 0.0061(10) 0.0028(10)
C31 0.036(5) 0.028(3) 0.023(4) -0.013(3) 0.004(4) -0.002(3)
C32 0.017(5) 0.046(4) 0.035(5) -0.014(4) -0.003(4) -0.001(3)
C33 0.053(7) 0.048(4) 0.029(5) -0.013(4) -0.003(4) -0.019(4)
C34 0.085(9) 0.037(4) 0.040(5) 0.006(4) -0.006(5) -0.003(4)
C35 0.068(8) 0.050(4) 0.033(5) -0.005(4) -0.008(5) -0.003(4)
C36 0.024(5) 0.049(4) 0.038(5) -0.017(4) 0.001(4) -0.013(4)
Cl41 0.0262(8) 0.0371(8) 0.0365(9) -0.0021(7) -0.0029(7) -0.0054(6)
C41 0.028(3) 0.014(3) 0.028(3) -0.006(2) -0.004(3) 0.002(2)
C42 0.043(4) 0.021(3) 0.022(4) -0.012(3) -0.007(3) 0.008(4)
C43 0.039(4) 0.021(3) 0.068(5) -0.012(3) -0.032(4) -0.001(3)
C45 0.054(4) 0.015(3) 0.030(4) -0.010(3) 0.007(3) -0.004(3)
C46 0.052(5) 0.016(3) 0.032(4) -0.001(3) -0.018(4) -0.003(4)

```

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All esds 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

Cl31 C31 1.785(4) . . yes

Cl41 C41 1.725(3) . . yes

O11 C171 1.211(3) . . yes

O12 C172 1.449(3) . . yes

O12 C171 1.331(3) . . yes

O21 C271 1.204(3) . . yes

O22 C272 1.458(4) . . yes

O22 C271 1.332(4) . . yes

C11 C161 1.501(3) . . no

C11 C12 1.630(3) . . no

C11 C16 1.489(3) . . no

C11 C19 1.489(3) . . no

C12 C161 1.514(3) . . no

C12 C13 1.491(4) . . no

C12 C112 1.489(3) . . no

C13 C114 1.443(3) . . no

C13 C14 1.381(3) . . no

C14 C117 1.449(4) . . no

C14 C15 1.475(3) . . no

C15 C119 1.450(4) . . no

C15 C16 1.375(3) . . no

C16 C17 1.436(3) . . no
C17 C18 1.449(3) . . no
C17 C121 1.386(4) . . no
C18 C19 1.438(3) . . no
C18 C124 1.395(4) . . no
C19 C110 1.382(3) . . no
C110 C126 1.452(3) . . no
C110 C111 1.475(3) . . no
C111 C112 1.374(3) . . no
C111 C128 1.450(3) . . no
C112 C113 1.440(3) . . no
C113 C114 1.441(3) . . no
C113 C130 1.387(3) . . no
C114 C115 1.389(4) . . no
C115 C132 1.453(3) . . no
C115 C116 1.444(4) . . no
C116 C134 1.442(4) . . no
C116 C117 1.393(3) . . no
C117 C118 1.443(4) . . no
C118 C119 1.446(3) . . no
C118 C136 1.392(4) . . no
C119 C120 1.396(4) . . no
C120 C138 1.450(4) . . no
C120 C121 1.429(4) . . no
C121 C122 1.450(4) . . no
C122 C139 1.445(4) . . no
C122 C123 1.383(4) . . no
C123 C142 1.455(4) . . no
C123 C124 1.453(4) . . no
C124 C125 1.442(4) . . no
C125 C126 1.389(4) . . no
C125 C143 1.447(4) . . no
C126 C127 1.448(4) . . no
C127 C128 1.439(4) . . no
C127 C145 1.394(4) . . no
C128 C129 1.389(3) . . no
C129 C147 1.457(4) . . no
C129 C130 1.433(3) . . no
C130 C131 1.449(4) . . no
C131 C148 1.449(4) . . no
C131 C132 1.386(4) . . no
C132 C133 1.450(4) . . no
C133 C134 1.450(4) . . no
C133 C150 1.393(4) . . no
C134 C135 1.386(4) . . no
C135 C152 1.455(4) . . no
C135 C136 1.446(4) . . no
C136 C137 1.451(4) . . no
C137 C138 1.392(4) . . no
C137 C153 1.453(4) . . no
C138 C139 1.444(4) . . no
C139 C140 1.389(4) . . no
C140 C154 1.446(4) . . no
C140 C141 1.448(4) . . no
C141 C160 1.451(3) . . no
C141 C142 1.389(4) . . no
C142 C143 1.454(4) . . no
C143 C144 1.390(4) . . no
C144 C159 1.440(4) . . no
C144 C145 1.448(4) . . no
C145 C146 1.453(4) . . no
C146 C158 1.449(4) . . no
C146 C147 1.387(3) . . no
C147 C148 1.449(4) . . no
C148 C149 1.390(4) . . no
C149 C150 1.451(4) . . no
C149 C157 1.450(3) . . no

C150 C151 1.449(3) . . no
C151 C156 1.452(3) . . no
C151 C152 1.391(4) . . no
C152 C153 1.450(4) . . no
C153 C154 1.381(4) . . no
C154 C155 1.460(4) . . no
C155 C156 1.394(4) . . no
C155 C160 1.447(4) . . no
C156 C157 1.446(4) . . no
C157 C158 1.385(4) . . no
C158 C159 1.451(4) . . no
C159 C160 1.387(4) . . no
C161 C162 1.506(3) . . no
C161 C168 1.526(4) . . no
C162 C163 1.393(4) . . no
C162 C167 1.390(3) . . no
C163 C164 1.380(4) . . no
C164 C165 1.386(4) . . no
C165 C166 1.382(4) . . no
C166 C167 1.390(4) . . no
C168 C169 1.528(4) . . no
C169 C170 1.524(4) . . no
C170 C171 1.506(4) . . no
C21 C26 1.484(4) . . no
C21 C22 1.625(3) . . no
C21 C29 1.489(3) . . no
C21 C261 1.515(3) . . no
C22 C23 1.483(4) . . no
C22 C261 1.525(3) . . no
C22 C212 1.488(3) . . no
C23 C214 1.445(3) . . no
C23 C24 1.379(3) . . no
C24 C217 1.448(4) . . no
C24 C25 1.471(3) . . no
C25 C219 1.452(4) . . no
C25 C26 1.377(4) . . no
C26 C27 1.445(3) . . no
C27 C28 1.444(4) . . no
C27 C221 1.393(4) . . no
C28 C29 1.443(3) . . no
C28 C224 1.392(3) . . no
C29 C210 1.377(3) . . no
C163 H163 0.9636 . . no
C164 H164 0.9883 . . no
C165 H165 0.9983 . . no
C166 H166 0.9993 . . no
C167 H167 1.0119 . . no
C168 H168 0.9651 . . no
C168 H168' 0.9936 . . no
C169 H169 1.0031 . . no
C169 H169' 1.0099 . . no
C170 H170 1.0491 . . no
C170 H170' 0.9894 . . no
C172 H172" 0.9996 . . no
C172 H172 1.0773 . . no
C172 H172' 1.0740 . . no
C210 C226 1.447(3) . . no
C210 C211 1.476(3) . . no
C211 C212 1.381(3) . . no
C211 C228 1.436(3) . . no
C212 C213 1.443(3) . . no
C213 C230 1.392(3) . . no
C213 C214 1.437(3) . . no
C214 C215 1.390(4) . . no
C215 C216 1.446(4) . . no
C215 C232 1.452(3) . . no
C216 C217 1.386(4) . . no

C216 C234 1.449(4) . . no
C217 C218 1.446(4) . . no
C218 C236 1.396(4) . . no
C218 C219 1.446(4) . . no
C219 C220 1.381(3) . . no
C220 C238 1.451(3) . . no
C220 C221 1.446(4) . . no
C221 C222 1.441(4) . . no
C222 C239 1.446(4) . . no
C222 C223 1.386(4) . . no
C223 C242 1.451(4) . . no
C223 C224 1.451(4) . . no
C224 C225 1.439(3) . . no
C225 C226 1.389(3) . . no
C225 C243 1.453(4) . . no
C226 C227 1.451(3) . . no
C227 C228 1.444(3) . . no
C227 C245 1.390(4) . . no
C228 C229 1.398(3) . . no
C229 C230 1.439(3) . . no
C229 C247 1.455(3) . . no
C230 C231 1.449(4) . . no
C231 C248 1.442(3) . . no
C31 C32 1.387(6) . . no
C31 C36 1.386(7) . . no
C231 C232 1.395(4) . . no
C32 C33 1.387(7) . . no
C232 C233 1.448(4) . . no
C233 C250 1.389(3) . . no
C33 C34 1.388(8) . . no
C233 C234 1.454(3) . . no
C234 C235 1.382(4) . . no
C34 C35 1.387(8) . . no
C235 C236 1.453(3) . . no
C235 C252 1.444(4) . . no
C35 C36 1.388(7) . . no
C236 C237 1.444(3) . . no
C237 C238 1.391(3) . . no
C237 C253 1.447(4) . . no
C238 C239 1.449(3) . . no
C239 C240 1.395(4) . . no
C240 C241 1.444(4) . . no
C240 C254 1.449(3) . . no
C241 C260 1.457(3) . . no
C241 C242 1.390(4) . . no
C242 C243 1.448(4) . . no
C243 C244 1.383(3) . . no
C244 C245 1.446(4) . . no
C244 C259 1.454(4) . . no
C245 C246 1.450(4) . . no
C246 C258 1.443(4) . . no
C246 C247 1.385(3) . . no
C247 C248 1.451(4) . . no
C248 C249 1.395(4) . . no
C249 C250 1.454(4) . . no
C249 C257 1.447(3) . . no
C250 C251 1.445(3) . . no
C251 C252 1.395(3) . . no
C251 C256 1.453(3) . . no
C252 C253 1.456(3) . . no
C253 C254 1.387(4) . . no
C254 C255 1.452(4) . . no
C255 C260 1.452(4) . . no
C255 C256 1.385(3) . . no
C256 C257 1.446(4) . . no
C257 C258 1.389(4) . . no
C258 C259 1.451(4) . . no

C259 C260 1.383(4) . . no
 C261 C262 1.509(3) . . no
 C261 C268 1.530(4) . . no
 C262 C263 1.386(4) . . no
 C262 C267 1.390(4) . . no
 C263 C264 1.387(4) . . no
 C264 C265 1.372(4) . . no
 C265 C266 1.385(4) . . no
 C266 C267 1.384(4) . . no
 C268 C269 1.531(4) . . no
 C269 C270 1.545(4) . . no
 C270 C271 1.497(4) . . no
 C32 H32 0.9502 . . no
 C33 H33 0.9499 . . no
 C34 H34 0.9500 . . no
 C35 H35 0.9494 . . no
 C36 H36 0.9502 . . no
 C263 H263 0.9624 . . no
 C264 H264 0.9396 . . no
 C265 H265 0.9552 . . no
 C266 H266 0.9795 . . no
 C267 H267 1.0040 . . no
 C268 H268' 1.0178 . . no
 C268 H268 1.0433 . . no
 C269 H269' 1.0565 . . no
 C269 H269 1.0197 . . no
 C270 H270 1.0208 . . no
 C270 H270' 0.9805 . . no
 C272 H272 0.9692 . . no
 C272 H272" 1.0334 . . no
 C272 H272' 1.0147 . . no
 C41 C42 1.385(5) . . no
 C41 C46 1.386(5) . . no
 C42 C43 1.385(5) . . no
 C43 C44 1.3838 . . no
 C44 C45 1.3846 . . no
 C45 C46 1.386(6) . . no
 C42 H42 0.9498 . . no
 C43 H43 0.9507 . . no
 C44 H44 0.9500 . . no
 C45 H45 0.9500 . . no
 C46 H46 0.9488 . . no

loop_

_geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 C171 O12 C172 116.1(2) . . . yes
 C271 O22 C272 115.5(3) . . . yes
 C12 C11 C16 114.85(19) . . . no
 C12 C11 C161 57.63(15) . . . no
 C16 C11 C19 104.85(19) . . . no
 C16 C11 C161 126.8(2) . . . no
 C19 C11 C161 126.7(2) . . . no
 C12 C11 C19 114.71(19) . . . no
 C11 C12 C112 115.44(19) . . . no
 C11 C12 C161 56.88(15) . . . no
 C11 C12 C13 115.2(2) . . . no
 C13 C12 C161 126.1(2) . . . no
 C112 C12 C161 127.2(2) . . . no
 C13 C12 C112 105.0(2) . . . no
 C12 C13 C14 123.5(2) . . . no

C14 C13 C114 119.2(2) . . . no
C12 C13 C114 108.2(2) . . . no
C13 C14 C15 120.8(2) . . . no
C15 C14 C117 107.1(2) . . . no
C13 C14 C117 120.0(2) . . . no
C14 C15 C119 107.5(2) . . . no
C16 C15 C119 119.8(2) . . . no
C14 C15 C16 121.1(2) . . . no
C11 C16 C15 123.7(2) . . . no
C15 C16 C17 119.4(2) . . . no
C11 C16 C17 108.4(2) . . . no
C16 C17 C18 108.3(2) . . . no
C18 C17 C121 120.3(2) . . . no
C16 C17 C121 121.4(2) . . . no
C17 C18 C19 108.7(2) . . . no
C17 C18 C124 119.7(2) . . . no
C19 C18 C124 121.0(2) . . . no
C11 C19 C18 108.1(2) . . . no
C11 C19 C110 123.6(2) . . . no
C18 C19 C110 119.3(2) . . . no
C19 C110 C126 120.2(2) . . . no
C111 C110 C126 107.2(2) . . . no
C19 C110 C111 121.1(2) . . . no
C110 C111 C112 120.8(2) . . . no
C112 C111 C128 120.0(2) . . . no
C110 C111 C128 107.6(2) . . . no
C12 C112 C111 123.5(2) . . . no
C111 C112 C113 119.5(2) . . . no
C12 C112 C113 108.1(2) . . . no
C112 C113 C114 108.9(2) . . . no
C112 C113 C130 121.0(2) . . . no
C114 C113 C130 120.2(2) . . . no
C13 C114 C113 108.4(2) . . . no
C13 C114 C115 121.4(2) . . . no
C113 C114 C115 120.0(2) . . . no
C114 C115 C132 119.9(2) . . . no
C116 C115 C132 108.2(2) . . . no
C114 C115 C116 119.3(2) . . . no
C115 C116 C134 108.1(2) . . . no
C117 C116 C134 120.0(2) . . . no
C115 C116 C117 119.5(2) . . . no
C14 C117 C118 108.8(2) . . . no
C116 C117 C118 119.9(2) . . . no
C14 C117 C116 120.5(2) . . . no
C117 C118 C136 119.9(2) . . . no
C119 C118 C136 120.1(2) . . . no
C117 C118 C119 108.1(2) . . . no
C15 C119 C118 108.4(2) . . . no
C118 C119 C120 120.2(2) . . . no
C15 C119 C120 120.2(2) . . . no
C119 C120 C121 119.7(2) . . . no
C121 C120 C138 107.8(2) . . . no
C119 C120 C138 119.7(2) . . . no
C17 C121 C122 120.3(2) . . . no
C120 C121 C122 108.6(2) . . . no
C17 C121 C120 119.4(2) . . . no
C121 C122 C139 107.6(2) . . . no
C123 C122 C139 120.1(2) . . . no
C121 C122 C123 119.5(2) . . . no
C122 C123 C142 119.8(2) . . . no
C124 C123 C142 107.6(2) . . . no
C122 C123 C124 120.7(2) . . . no
C18 C124 C123 119.6(2) . . . no
C123 C124 C125 108.4(2) . . . no
C18 C124 C125 119.5(2) . . . no
C124 C125 C126 119.6(2) . . . no
C126 C125 C143 120.3(2) . . . no

C124	C125	C143	108.0(2)	.	.	.	no
C110	C126	C127	108.2(2)	.	.	.	no
C125	C126	C127	119.6(2)	.	.	.	no
C110	C126	C125	120.3(2)	.	.	.	no
C126	C127	C128	108.5(2)	.	.	.	no
C128	C127	C145	120.6(2)	.	.	.	no
C126	C127	C145	119.9(2)	.	.	.	no
C111	C128	C127	108.4(2)	.	.	.	no
C127	C128	C129	120.0(2)	.	.	.	no
C111	C128	C129	119.9(2)	.	.	.	no
C128	C129	C130	120.2(2)	.	.	.	no
C128	C129	C147	119.6(2)	.	.	.	no
C130	C129	C147	107.3(2)	.	.	.	no
C113	C130	C129	119.3(2)	.	.	.	no
C113	C130	C131	120.0(2)	.	.	.	no
C129	C130	C131	109.0(2)	.	.	.	no
C130	C131	C148	107.7(2)	.	.	.	no
C132	C131	C148	120.1(2)	.	.	.	no
C130	C131	C132	119.9(2)	.	.	.	no
C115	C132	C131	120.0(2)	.	.	.	no
C131	C132	C133	120.2(2)	.	.	.	no
C115	C132	C133	107.6(2)	.	.	.	no
C132	C133	C134	108.0(2)	.	.	.	no
C134	C133	C150	120.3(2)	.	.	.	no
C132	C133	C150	119.6(2)	.	.	.	no
C116	C134	C133	108.1(2)	.	.	.	no
C116	C134	C135	120.2(2)	.	.	.	no
C133	C134	C135	119.7(2)	.	.	.	no
C134	C135	C136	119.9(2)	.	.	.	no
C134	C135	C152	120.1(2)	.	.	.	no
C136	C135	C152	107.7(2)	.	.	.	no
C118	C136	C137	119.8(2)	.	.	.	no
C135	C136	C137	108.3(2)	.	.	.	no
C118	C136	C135	120.1(2)	.	.	.	no
C136	C137	C153	108.0(2)	.	.	.	no
C138	C137	C153	119.9(2)	.	.	.	no
C136	C137	C138	120.2(2)	.	.	.	no
C120	C138	C137	120.0(2)	.	.	.	no
C137	C138	C139	120.0(2)	.	.	.	no
C120	C138	C139	108.2(2)	.	.	.	no
C122	C139	C138	107.8(2)	.	.	.	no
C138	C139	C140	120.0(2)	.	.	.	no
C122	C139	C140	120.4(2)	.	.	.	no
C139	C140	C141	119.6(2)	.	.	.	no
C139	C140	C154	120.0(2)	.	.	.	no
C141	C140	C154	108.0(2)	.	.	.	no
C140	C141	C142	120.2(2)	.	.	.	no
C140	C141	C160	108.2(2)	.	.	.	no
C142	C141	C160	119.7(2)	.	.	.	no
C123	C142	C143	107.8(2)	.	.	.	no
C141	C142	C143	120.4(2)	.	.	.	no
C123	C142	C141	119.9(2)	.	.	.	no
C125	C143	C142	108.1(2)	.	.	.	no
C142	C143	C144	119.2(2)	.	.	.	no
C125	C143	C144	120.3(2)	.	.	.	no
C143	C144	C145	119.3(2)	.	.	.	no
C145	C144	C159	108.3(2)	.	.	.	no
C143	C144	C159	120.7(2)	.	.	.	no
C127	C145	C144	120.5(2)	.	.	.	no
C127	C145	C146	119.6(2)	.	.	.	no
C144	C145	C146	107.7(2)	.	.	.	no
C145	C146	C147	119.7(2)	.	.	.	no
C145	C146	C158	108.0(2)	.	.	.	no
C147	C146	C158	120.0(2)	.	.	.	no
C129	C147	C148	108.3(2)	.	.	.	no
C146	C147	C148	119.8(2)	.	.	.	no
C129	C147	C146	120.4(2)	.	.	.	no

C131	C148	C147	107.6(2)	.	.	.	no
C131	C148	C149	120.0(2)	.	.	.	no
C147	C148	C149	119.9(2)	.	.	.	no
C148	C149	C150	119.8(2)	.	.	.	no
C148	C149	C157	120.5(2)	.	.	.	no
C150	C149	C157	107.9(2)	.	.	.	no
C133	C150	C151	120.0(2)	.	.	.	no
C149	C150	C151	108.0(2)	.	.	.	no
C133	C150	C149	120.2(2)	.	.	.	no
C150	C151	C156	108.0(2)	.	.	.	no
C152	C151	C156	120.0(2)	.	.	.	no
C150	C151	C152	119.8(2)	.	.	.	no
C135	C152	C153	108.2(2)	.	.	.	no
C151	C152	C153	119.8(2)	.	.	.	no
C135	C152	C151	120.0(2)	.	.	.	no
C137	C153	C152	107.7(2)	.	.	.	no
C137	C153	C154	119.8(2)	.	.	.	no
C152	C153	C154	120.8(2)	.	.	.	no
C140	C154	C153	120.3(2)	.	.	.	no
C140	C154	C155	107.9(2)	.	.	.	no
C153	C154	C155	119.5(2)	.	.	.	no
C154	C155	C160	107.9(2)	.	.	.	no
C156	C155	C160	120.3(2)	.	.	.	no
C154	C155	C156	119.9(2)	.	.	.	no
C151	C156	C157	108.0(2)	.	.	.	no
C155	C156	C157	119.5(2)	.	.	.	no
C151	C156	C155	120.0(2)	.	.	.	no
C149	C157	C158	119.2(2)	.	.	.	no
C156	C157	C158	120.3(2)	.	.	.	no
C149	C157	C156	108.1(2)	.	.	.	no
C146	C158	C159	107.8(2)	.	.	.	no
C157	C158	C159	120.1(2)	.	.	.	no
C146	C158	C157	120.6(2)	.	.	.	no
C144	C159	C158	108.2(2)	.	.	.	no
C158	C159	C160	119.9(2)	.	.	.	no
C144	C159	C160	120.1(2)	.	.	.	no
C141	C160	C155	107.9(2)	.	.	.	no
C155	C160	C159	119.9(2)	.	.	.	no
C141	C160	C159	120.0(2)	.	.	.	no
C11	C161	C12	65.48(16)	.	.	.	no
C11	C161	C162	119.9(2)	.	.	.	no
C12	C161	C162	117.0(2)	.	.	.	no
C12	C161	C168	116.3(2)	.	.	.	no
C11	C161	C168	117.3(2)	.	.	.	no
C162	C161	C168	113.0(2)	.	.	.	no
C161	C162	C167	122.7(2)	.	.	.	no
C163	C162	C167	118.7(2)	.	.	.	no
C161	C162	C163	118.5(2)	.	.	.	no
C162	C163	C164	120.8(2)	.	.	.	no
C163	C164	C165	120.2(2)	.	.	.	no
C164	C165	C166	119.6(2)	.	.	.	no
C165	C166	C167	120.3(2)	.	.	.	no
C162	C167	C166	120.4(2)	.	.	.	no
C161	C168	C169	112.7(2)	.	.	.	no
C168	C169	C170	109.6(2)	.	.	.	no
C169	C170	C171	113.5(2)	.	.	.	no
O11	C171	C170	125.3(2)	.	.	.	yes
O12	C171	C170	111.1(2)	.	.	.	yes
O11	C171	O12	123.6(2)	.	.	.	yes
C22	C21	C26	115.4(2)	.	.	.	no
C22	C21	C29	114.45(19)	.	.	.	no
C22	C21	C261	57.98(15)	.	.	.	no
C26	C21	C29	105.22(19)	.	.	.	no
C26	C21	C261	126.8(2)	.	.	.	no
C29	C21	C261	126.1(2)	.	.	.	no
C21	C22	C23	114.7(2)	.	.	.	no
C21	C22	C212	115.45(19)	.	.	.	no

C21 C22 C261 57.37(15) . . . no
C23 C22 C212 104.96(19) . . . no
C23 C22 C261 126.4(2) . . . no
C212 C22 C261 126.9(2) . . . no
C22 C23 C24 123.8(2) . . . no
C22 C23 C214 108.2(2) . . . no
C24 C23 C214 119.3(2) . . . no
C23 C24 C25 121.0(2) . . . no
C23 C24 C217 119.7(2) . . . no
C25 C24 C217 107.3(2) . . . no
C24 C25 C26 120.6(2) . . . no
C24 C25 C219 107.7(2) . . . no
C26 C25 C219 119.5(2) . . . no
C21 C26 C25 123.6(2) . . . no
C21 C26 C27 108.1(2) . . . no
C25 C26 C27 119.4(2) . . . no
C26 C27 C28 108.6(2) . . . no
C26 C27 C221 121.2(2) . . . no
C28 C27 C221 120.1(2) . . . no
C27 C28 C29 108.4(2) . . . no
C27 C28 C224 120.1(2) . . . no
C29 C28 C224 121.3(2) . . . no
C21 C29 C210 124.2(2) . . . no
C28 C29 C210 118.7(2) . . . no
C21 C29 C28 108.1(2) . . . no
C162 C163 H163 121.20 . . . no
C164 C163 H163 117.97 . . . no
C163 C164 H164 120.03 . . . no
C165 C164 H164 119.76 . . . no
C166 C165 H165 120.12 . . . no
C164 C165 H165 120.16 . . . no
C165 C166 H166 119.63 . . . no
C167 C166 H166 120.08 . . . no
C162 C167 H167 120.37 . . . no
C166 C167 H167 119.18 . . . no
C169 C168 H168' 105.33 . . . no
H168' C168 H168 112.06 . . . no
C161 C168 H168 108.81 . . . no
C169 C168 H168 108.02 . . . no
C161 C168 H168' 109.90 . . . no
C168 C169 H169' 111.33 . . . no
H169' C169 H169 110.26 . . . no
C170 C169 H169 110.33 . . . no
C168 C169 H169 108.29 . . . no
C170 C169 H169' 107.07 . . . no
C169 C170 H170' 107.38 . . . no
C169 C170 H170 106.81 . . . no
C171 C170 H170' 107.85 . . . no
C171 C170 H170 109.37 . . . no
H170' C170 H170 111.93 . . . no
O12 C172 H172 111.21 . . . no
H172' C172 H172 113.43 . . . no
H172" C172 H172 101.69 . . . no
H172' C172 H172" 115.88 . . . no
O12 C172 H172' 104.02 . . . no
O12 C172 H172" 110.84 . . . no
C29 C210 C211 120.9(2) . . . no
C29 C210 C226 120.4(2) . . . no
C211 C210 C226 107.3(2) . . . no
C210 C211 C212 120.4(2) . . . no
C210 C211 C228 107.6(2) . . . no
C212 C211 C228 120.1(2) . . . no
C22 C212 C211 123.8(2) . . . no
C22 C212 C213 108.3(2) . . . no
C211 C212 C213 119.1(2) . . . no
C212 C213 C214 108.4(2) . . . no
C212 C213 C230 121.4(2) . . . no

C214 C213 C230 120.3(2) . . . no
C23 C214 C213 108.7(2) . . . no
C23 C214 C215 121.3(2) . . . no
C213 C214 C215 120.1(2) . . . no
C214 C215 C216 119.0(2) . . . no
C214 C215 C232 119.9(2) . . . no
C216 C215 C232 108.5(2) . . . no
C215 C216 C217 119.5(2) . . . no
C215 C216 C234 107.5(2) . . . no
C217 C216 C234 120.4(2) . . . no
C24 C217 C216 121.0(2) . . . no
C24 C217 C218 108.6(2) . . . no
C216 C217 C218 119.5(2) . . . no
C217 C218 C219 108.2(2) . . . no
C217 C218 C236 120.5(2) . . . no
C219 C218 C236 119.8(2) . . . no
C25 C219 C218 108.2(2) . . . no
C25 C219 C220 121.2(2) . . . no
C218 C219 C220 120.1(2) . . . no
C219 C220 C221 119.5(2) . . . no
C219 C220 C238 120.4(2) . . . no
C221 C220 C238 107.0(2) . . . no
C27 C221 C220 119.1(2) . . . no
C27 C221 C222 119.6(2) . . . no
C220 C221 C222 109.2(2) . . . no
C221 C222 C223 120.8(2) . . . no
C221 C222 C239 107.5(2) . . . no
C223 C222 C239 119.6(2) . . . no
C222 C223 C224 119.5(2) . . . no
C222 C223 C242 120.8(2) . . . no
C224 C223 C242 107.6(2) . . . no
C28 C224 C223 119.9(2) . . . no
C28 C224 C225 119.5(2) . . . no
C223 C224 C225 108.6(2) . . . no
C224 C225 C226 119.2(2) . . . no
C224 C225 C243 107.7(2) . . . no
C226 C225 C243 120.3(2) . . . no
C210 C226 C225 120.6(2) . . . no
C210 C226 C227 108.3(2) . . . no
C225 C226 C227 119.6(2) . . . no
C226 C227 C228 107.9(2) . . . no
C226 C227 C245 119.9(2) . . . no
C228 C227 C245 120.6(2) . . . no
C211 C228 C227 108.8(2) . . . no
C211 C228 C229 120.7(2) . . . no
C227 C228 C229 119.5(2) . . . no
C228 C229 C230 119.5(2) . . . no
C228 C229 C247 120.0(2) . . . no
C230 C229 C247 107.9(2) . . . no
C213 C230 C229 119.1(2) . . . no
C213 C230 C231 120.0(2) . . . no
C229 C230 C231 108.4(2) . . . no
C230 C231 C232 119.6(2) . . . no
C230 C231 C248 107.9(2) . . . no
C232 C231 C248 120.1(2) . . . no
C32 C31 C36 120.0(4) . . . no
C131 C31 C32 119.1(3) . . . yes
C131 C31 C36 121.0(3) . . . yes
C215 C232 C231 120.0(2) . . . no
C215 C232 C233 108.0(2) . . . no
C231 C232 C233 119.7(2) . . . no
C31 C32 C33 120.0(4) . . . no
C232 C233 C234 107.6(2) . . . no
C32 C33 C34 120.0(5) . . . no
C234 C233 C250 120.1(2) . . . no
C232 C233 C250 120.4(2) . . . no
C216 C234 C233 108.5(2) . . . no

C33 C34 C35 120.0(5) . . . no
C216 C234 C235 120.2(2) . . . no
C233 C234 C235 120.0(2) . . . no
C234 C235 C252 119.9(2) . . . no
C234 C235 C236 120.0(2) . . . no
C34 C35 C36 119.9(5) . . . no
C236 C235 C252 107.8(2) . . . no
C31 C36 C35 120.0(5) . . . no
C218 C236 C235 119.5(2) . . . no
C218 C236 C237 120.0(2) . . . no
C235 C236 C237 108.3(2) . . . no
C236 C237 C253 108.0(2) . . . no
C238 C237 C253 119.9(2) . . . no
C236 C237 C238 120.1(2) . . . no
C220 C238 C237 119.6(2) . . . no
C237 C238 C239 120.0(2) . . . no
C220 C238 C239 108.2(2) . . . no
C222 C239 C240 120.0(2) . . . no
C238 C239 C240 120.1(2) . . . no
C222 C239 C238 108.1(2) . . . no
C239 C240 C241 120.1(2) . . . no
C239 C240 C254 119.6(2) . . . no
C241 C240 C254 108.2(2) . . . no
C240 C241 C242 120.2(2) . . . no
C240 C241 C260 108.0(2) . . . no
C242 C241 C260 119.5(2) . . . no
C223 C242 C241 119.3(2) . . . no
C223 C242 C243 107.9(2) . . . no
C241 C242 C243 120.2(2) . . . no
C225 C243 C242 108.1(2) . . . no
C225 C243 C244 119.7(2) . . . no
C242 C243 C244 120.1(2) . . . no
C243 C244 C259 120.2(2) . . . no
C245 C244 C259 107.8(2) . . . no
C243 C244 C245 120.2(2) . . . no
C227 C245 C244 120.2(2) . . . no
C227 C245 C246 119.8(2) . . . no
C244 C245 C246 108.2(2) . . . no
C245 C246 C247 120.2(2) . . . no
C245 C246 C258 108.0(2) . . . no
C247 C246 C258 119.8(2) . . . no
C229 C247 C248 107.7(2) . . . no
C229 C247 C246 119.9(2) . . . no
C246 C247 C248 120.3(2) . . . no
C247 C248 C249 119.4(2) . . . no
C231 C248 C247 108.1(2) . . . no
C231 C248 C249 120.3(2) . . . no
C248 C249 C257 120.4(2) . . . no
C250 C249 C257 107.7(2) . . . no
C248 C249 C250 119.7(2) . . . no
C233 C250 C251 119.9(2) . . . no
C249 C250 C251 108.0(2) . . . no
C233 C250 C249 119.9(2) . . . no
C250 C251 C256 108.2(2) . . . no
C252 C251 C256 120.0(2) . . . no
C250 C251 C252 119.7(2) . . . no
C235 C252 C251 120.3(2) . . . no
C235 C252 C253 108.0(2) . . . no
C251 C252 C253 119.6(2) . . . no
C237 C253 C252 107.9(2) . . . no
C237 C253 C254 120.2(2) . . . no
C252 C253 C254 120.2(2) . . . no
C240 C254 C253 120.3(2) . . . no
C253 C254 C255 119.9(2) . . . no
C240 C254 C255 108.0(2) . . . no
C254 C255 C260 108.0(2) . . . no
C256 C255 C260 119.8(2) . . . no

C254	C255	C256	120.3(2)	.	.	.	no
C251	C256	C257	107.7(2)	.	.	.	no
C255	C256	C257	120.4(2)	.	.	.	no
C251	C256	C255	120.0(2)	.	.	.	no
C249	C257	C258	119.5(2)	.	.	.	no
C256	C257	C258	119.8(2)	.	.	.	no
C249	C257	C256	108.4(2)	.	.	.	no
C257	C258	C259	119.8(2)	.	.	.	no
C246	C258	C257	120.6(2)	.	.	.	no
C246	C258	C259	108.1(2)	.	.	.	no
C244	C259	C260	119.7(2)	.	.	.	no
C258	C259	C260	120.2(2)	.	.	.	no
C244	C259	C258	107.8(2)	.	.	.	no
C241	C260	C259	120.3(2)	.	.	.	no
C255	C260	C259	120.0(2)	.	.	.	no
C241	C260	C255	107.8(2)	.	.	.	no
C21	C261	C22	64.66(16)	.	.	.	no
C21	C261	C262	118.9(2)	.	.	.	no
C22	C261	C262	115.1(2)	.	.	.	no
C22	C261	C268	117.9(2)	.	.	.	no
C21	C261	C268	115.9(2)	.	.	.	no
C262	C261	C268	115.1(2)	.	.	.	no
C261	C262	C263	121.9(2)	.	.	.	no
C261	C262	C267	119.0(2)	.	.	.	no
C263	C262	C267	119.0(2)	.	.	.	no
C262	C263	C264	120.0(2)	.	.	.	no
C263	C264	C265	120.6(3)	.	.	.	no
C264	C265	C266	119.9(3)	.	.	.	no
C265	C266	C267	119.7(3)	.	.	.	no
C262	C267	C266	120.7(2)	.	.	.	no
C261	C268	C269	113.0(2)	.	.	.	no
C268	C269	C270	112.7(2)	.	.	.	no
C269	C270	C271	113.4(2)	.	.	.	no
O21	C271	C270	125.5(3)	.	.	.	yes
O22	C271	C270	111.6(2)	.	.	.	yes
O21	C271	O22	122.9(3)	.	.	.	yes
C31	C32	H32	119.98	.	.	.	no
C33	C32	H32	120.01	.	.	.	no
C32	C33	H33	120.00	.	.	.	no
C34	C33	H33	120.02	.	.	.	no
C33	C34	H34	119.97	.	.	.	no
C35	C34	H34	119.99	.	.	.	no
C34	C35	H35	120.07	.	.	.	no
C36	C35	H35	119.99	.	.	.	no
C31	C36	H36	120.00	.	.	.	no
C35	C36	H36	119.95	.	.	.	no
C264	C263	H263	121.02	.	.	.	no
C262	C263	H263	118.89	.	.	.	no
C265	C264	H264	118.88	.	.	.	no
C263	C264	H264	120.48	.	.	.	no
C264	C265	H265	123.19	.	.	.	no
C266	C265	H265	116.85	.	.	.	no
C267	C266	H266	119.06	.	.	.	no
C265	C266	H266	121.26	.	.	.	no
C266	C267	H267	118.63	.	.	.	no
C262	C267	H267	120.47	.	.	.	no
C261	C268	H268	107.10	.	.	.	no
C261	C268	H268'	109.82	.	.	.	no
H268'	C268	H268	107.03	.	.	.	no
C269	C268	H268'	110.55	.	.	.	no
C269	C268	H268	109.11	.	.	.	no
C270	C269	H269	111.19	.	.	.	no
H269'	C269	H269	105.85	.	.	.	no
C270	C269	H269'	108.74	.	.	.	no
C268	C269	H269'	110.96	.	.	.	no
C268	C269	H269	107.15	.	.	.	no
C269	C270	H270'	106.12	.	.	.	no

C269 C270 H270 110.83 . . . no
 C271 C270 H270' 105.55 . . . no
 C271 C270 H270 106.74 . . . no
 H270' C270 H270 114.25 . . . no
 O22 C272 H272 107.49 . . . no
 H272' C272 H272 109.23 . . . no
 H272" C272 H272 112.80 . . . no
 H272' C272 H272" 110.35 . . . no
 O22 C272 H272' 105.84 . . . no
 O22 C272 H272" 110.84 . . . no
 C141 C41 C42 120.7(3) . . . yes
 C141 C41 C46 119.3(3) . . . yes
 C42 C41 C46 120.0(3) . . . no
 C41 C42 C43 120.0(3) . . . no
 C42 C43 C44 120.07 . . . no
 C43 C44 C45 119.99 . . . no
 C44 C45 C46 120.04 . . . no
 C41 C46 C45 119.9(3) . . . no
 C41 C42 H42 120.03 . . . no
 C43 C42 H42 120.00 . . . no
 C42 C43 H43 119.96 . . . no
 C44 C43 H43 119.98 . . . no
 C43 C44 H44 120.03 . . . no
 C45 C44 H44 119.98 . . . no
 C44 C45 H45 120.04 . . . no
 C46 C45 H45 119.92 . . . no
 C41 C46 H46 119.99 . . . no
 C45 C46 H46 120.08 . . . no

loop_

_geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
 C172 O12 C171 O11 -3.6(4) no
 C172 O12 C171 C170 176.2(2) no
 C272 O22 C271 O21 -4.9(4) no
 C272 O22 C271 C270 174.3(3) no
 C16 C11 C12 C112 121.5(2) no
 C12 C11 C16 C15 8.5(3) no
 C19 C11 C12 C112 -0.1(3) no
 C19 C11 C16 C17 -12.2(3) no
 C16 C11 C12 C161 -119.2(2) no
 C19 C11 C12 C13 -122.8(2) no
 C16 C11 C12 C13 -1.2(3) no
 C12 C11 C19 C110 -7.2(3) no
 C16 C11 C19 C18 12.5(3) no
 C16 C11 C19 C110 -134.1(2) no
 C161 C11 C19 C18 -153.7(2) no
 C161 C11 C19 C110 59.7(4) no
 C12 C11 C161 C162 -108.2(2) no
 C12 C11 C161 C168 108.2(2) no
 C16 C11 C161 C12 98.5(3) no
 C16 C11 C161 C162 -9.7(4) no
 C16 C11 C161 C168 -153.3(2) no
 C19 C11 C161 C12 -98.3(3) no
 C19 C11 C161 C162 153.5(2) no
 C161 C11 C16 C15 -58.5(3) no
 C161 C11 C16 C17 153.9(2) no
 C12 C11 C19 C18 139.4(2) no
 C19 C11 C161 C168 9.9(3) no

C161 C11 C12 C112 -119.3(2) no
C19 C11 C16 C15 135.4(2) no
C19 C11 C12 C161 119.2(2) no
C12 C11 C16 C17 -139.1(2) no
C161 C11 C12 C13 118.0(2) no
C161 C12 C13 C14 59.4(4) no
C161 C12 C13 C114 -154.1(2) no
C112 C12 C13 C114 11.6(3) no
C112 C12 C161 C11 98.5(3) no
C112 C12 C161 C162 -148.9(2) no
C11 C12 C161 C162 112.5(2) no
C11 C12 C161 C168 -109.7(2) no
C11 C12 C112 C113 -139.5(2) no
C13 C12 C112 C113 -11.6(3) no
C112 C12 C13 C14 -134.8(2) no
C11 C12 C13 C14 -6.7(3) no
C11 C12 C13 C114 139.7(2) no
C11 C12 C112 C111 7.5(4) no
C13 C12 C112 C111 135.4(3) no
C161 C12 C112 C111 -59.0(4) no
C112 C12 C161 C168 -11.2(3) no
C161 C12 C112 C113 154.0(2) no
C13 C12 C161 C11 -98.8(3) no
C13 C12 C161 C162 13.7(3) no
C13 C12 C161 C168 151.5(2) no
C114 C13 C14 C15 -135.2(2) no
C114 C13 C14 C117 2.4(3) no
C12 C13 C14 C117 145.5(2) no
C12 C13 C14 C15 7.8(4) no
C12 C13 C114 C113 -7.5(3) no
C14 C13 C114 C115 -4.6(4) no
C12 C13 C114 C115 -152.7(2) no
C14 C13 C114 C113 140.6(2) no
C13 C14 C117 C116 0.7(3) no
C117 C14 C15 C16 -142.5(2) no
C117 C14 C15 C119 0.4(2) no
C13 C14 C15 C119 142.8(2) no
C15 C14 C117 C116 143.4(2) no
C13 C14 C117 C118 -143.7(2) no
C13 C14 C15 C16 -0.1(4) no
C15 C14 C117 C118 -0.9(2) no
C119 C15 C16 C11 -146.9(2) no
C14 C15 C16 C17 135.9(2) no
C16 C15 C119 C120 -0.2(3) no
C14 C15 C16 C11 -8.3(4) no
C119 C15 C16 C17 -2.6(3) no
C14 C15 C119 C120 -143.7(2) no
C14 C15 C119 C118 0.2(3) no
C16 C15 C119 C118 143.7(2) no
C11 C16 C17 C121 153.0(2) no
C15 C16 C17 C121 3.8(3) no
C11 C16 C17 C18 7.6(3) no
C15 C16 C17 C18 -141.7(2) no
C16 C17 C121 C122 -141.0(2) no
C121 C17 C18 C124 -0.6(3) no
C18 C17 C121 C122 0.5(3) no
C16 C17 C18 C124 145.3(2) no
C121 C17 C18 C19 -145.5(2) no
C18 C17 C121 C120 139.4(2) no
C16 C17 C121 C120 -2.1(4) no
C16 C17 C18 C19 0.4(3) no
C17 C18 C124 C125 -137.6(2) no
C17 C18 C19 C11 -8.2(3) no
C124 C18 C19 C11 -152.6(2) no
C19 C18 C124 C125 3.0(4) no
C19 C18 C124 C123 140.6(2) no
C17 C18 C124 C123 0.1(3) no

C17 C18 C19 C110 140.0(2) no
C124 C18 C19 C110 -4.3(4) no
C18 C19 C110 C126 3.2(4) no
C18 C19 C110 C111 -135.5(2) no
C11 C19 C110 C126 146.3(2) no
C11 C19 C110 C111 7.6(4) no
C261 C21 C29 C210 60.1(4) no
C29 C21 C261 C22 -98.5(3) no
C29 C21 C261 C262 155.5(2) no
C22 C21 C261 C262 -106.0(2) no
C22 C21 C261 C268 110.2(2) no
C26 C21 C261 C22 99.5(3) no
C26 C21 C261 C262 -6.5(4) no
C26 C21 C261 C268 -150.3(2) no
C26 C21 C22 C23 -0.3(3) no
C26 C21 C22 C212 122.0(2) no
C26 C21 C22 C261 -119.0(2) no
C29 C21 C22 C23 -122.6(2) no
C29 C21 C22 C212 -0.3(3) no
C29 C21 C22 C261 118.7(2) no
C261 C21 C22 C23 118.7(2) no
C261 C21 C22 C212 -119.0(2) no
C22 C21 C26 C25 7.8(3) no
C22 C21 C26 C27 -138.9(2) no
C29 C21 C26 C25 135.0(2) no
C29 C21 C26 C27 -11.8(3) no
C261 C21 C26 C25 -60.0(3) no
C261 C21 C26 C27 153.2(2) no
C22 C21 C29 C28 139.6(2) no
C22 C21 C29 C210 -7.0(3) no
C26 C21 C29 C28 11.8(3) no
C26 C21 C29 C210 -134.8(2) no
C261 C21 C29 C28 -153.3(2) no
C29 C21 C261 C268 11.7(3) no
C21 C22 C261 C268 -107.2(2) no
C23 C22 C261 C21 -98.4(3) no
C21 C22 C212 C211 7.6(3) no
C23 C22 C212 C211 135.0(2) no
C261 C22 C212 C211 -59.4(4) no
C21 C22 C212 C213 -139.2(2) no
C23 C22 C212 C213 -11.8(3) no
C261 C22 C212 C213 153.7(2) no
C23 C22 C261 C262 13.3(3) no
C212 C22 C23 C24 -135.2(2) no
C212 C22 C23 C214 11.8(3) no
C261 C22 C23 C24 59.1(3) no
C261 C22 C23 C214 -153.9(2) no
C21 C22 C261 C262 111.7(2) no
C23 C22 C261 C268 154.4(2) no
C212 C22 C261 C21 99.1(3) no
C212 C22 C261 C262 -149.3(2) no
C212 C22 C261 C268 -8.1(3) no
C21 C22 C23 C24 -7.4(3) no
C21 C22 C23 C214 139.6(2) no
C24 C23 C214 C215 -4.5(3) no
C214 C23 C24 C217 2.4(3) no
C214 C23 C24 C25 -135.5(2) no
C22 C23 C214 C215 -153.2(2) no
C22 C23 C214 C213 -7.5(3) no
C24 C23 C214 C213 141.2(2) no
C22 C23 C24 C25 8.1(4) no
C22 C23 C24 C217 146.0(2) no
C217 C24 C25 C219 -0.4(3) no
C217 C24 C25 C26 -142.6(2) no
C25 C24 C217 C216 143.6(2) no
C23 C24 C25 C219 142.0(2) no
C23 C24 C217 C216 0.5(4) no

C25 C24 C217 C218 -0.2(3) no
C23 C24 C25 C26 -0.1(3) no
C23 C24 C217 C218 -143.3(2) no
C219 C25 C26 C27 -2.6(3) no
C24 C25 C26 C27 135.2(2) no
C26 C25 C219 C220 -1.0(4) no
C24 C25 C26 C21 -8.0(4) no
C219 C25 C26 C21 -145.8(2) no
C26 C25 C219 C218 143.5(2) no
C24 C25 C219 C220 -143.6(2) no
C24 C25 C219 C218 0.9(3) no
C25 C26 C27 C28 -140.9(2) no
C21 C26 C27 C221 152.9(2) no
C25 C26 C27 C221 4.5(3) no
C21 C26 C27 C28 7.5(3) no
C28 C27 C221 C222 0.4(3) no
C26 C27 C28 C29 0.1(3) no
C26 C27 C28 C224 145.8(2) no
C221 C27 C28 C224 0.0(4) no
C28 C27 C221 C220 138.8(2) no
C26 C27 C221 C222 -141.1(2) no
C221 C27 C28 C29 -145.8(2) no
C26 C27 C221 C220 -2.8(3) no
C224 C28 C29 C21 -152.8(2) no
C224 C28 C29 C210 -4.1(4) no
C27 C28 C29 C210 141.2(2) no
C27 C28 C29 C21 -7.6(3) no
C27 C28 C224 C225 -138.9(2) no
C29 C28 C224 C225 2.4(4) no
C29 C28 C224 C223 140.9(2) no
C27 C28 C224 C223 -0.4(3) no
C28 C29 C210 C211 -135.9(2) no
C28 C29 C210 C226 2.9(4) no
C21 C29 C210 C211 7.5(4) no
C21 C29 C210 C226 146.3(2) no
C12 C161 C168 H168 33.56 no
C162 C161 C168 H168' 49.87 no
C11 C161 C168 H168' -164.09 no
C162 C161 C168 H168 172.92 no
C12 C161 C168 H168' -89.48 no
C11 C161 C168 H168 -41.05 no
C161 C162 C163 H163 -3.47 no
C167 C162 C163 H163 -179.49 no
C161 C162 C167 H167 3.47 no
C163 C162 C167 H167 179.32 no
H163 C163 C164 C165 -179.43 no
C162 C163 C164 H164 178.96 no
H163 C163 C164 H164 -1.85 no
H164 C164 C165 C166 -178.85 no
H164 C164 C165 H165 5.27 no
C163 C164 C165 H165 -177.14 no
C164 C165 C166 H166 179.53 no
H165 C165 C166 H166 -4.60 no
H165 C165 C166 C167 175.99 no
H166 C166 C167 H167 1.38 no
H166 C166 C167 C162 -178.47 no
C165 C166 C167 H167 -179.21 no
H168' C168 C169 H169' -63.08 no
H168 C168 C169 C170 -64.76 no
H168 C168 C169 H169 55.62 no
H168' C168 C169 H169 175.54 no
C161 C168 C169 H169' 56.75 no
C161 C168 C169 H169 -64.63 no
H168 C168 C169 H169' 177.00 no
H168' C168 C169 C170 55.16 no
C168 C169 C170 H170 -57.41 no
H169 C169 C170 H170 -176.55 no

C168 C169 C170 H170' 62.82 no
H169 C169 C170 H170' -56.31 no
H169' C169 C170 C171 -57.19 no
H169 C169 C170 C171 62.81 no
H169' C169 C170 H170' -176.32 no
H169' C169 C170 H170 63.45 no
H170 C170 C171 O12 -45.90 no
H170' C170 C171 O11 11.88 no
H170' C170 C171 O12 -167.85 no
H170 C170 C171 O11 133.83 no
C226 C210 C211 C212 -143.3(2) no
C29 C210 C226 C225 -0.2(4) no
C211 C210 C226 C225 143.5(2) no
C211 C210 C226 C227 0.2(3) no
C29 C210 C211 C228 143.1(2) no
C226 C210 C211 C228 -0.4(3) no
C29 C210 C226 C227 -143.5(2) no
C29 C210 C211 C212 0.2(4) no
C212 C211 C228 C227 143.5(2) no
C228 C211 C212 C22 -146.2(2) no
C210 C211 C228 C229 -143.3(2) no
C210 C211 C212 C213 135.6(2) no
C210 C211 C228 C227 0.4(3) no
C210 C211 C212 C22 -7.9(4) no
C212 C211 C228 C229 -0.3(4) no
C228 C211 C212 C213 -2.7(3) no
C22 C212 C213 C230 153.2(2) no
C211 C212 C213 C214 -141.0(2) no
C22 C212 C213 C214 7.6(3) no
C211 C212 C213 C230 4.6(4) no
C230 C213 C214 C215 0.1(3) no
C214 C213 C230 C231 0.8(3) no
C212 C213 C230 C229 -3.3(4) no
C212 C213 C214 C23 -0.1(3) no
C214 C213 C230 C229 138.3(2) no
C230 C213 C214 C23 -146.1(2) no
C212 C213 C214 C215 146.2(2) no
C212 C213 C230 C231 -140.9(2) no
C213 C214 C215 C216 -138.4(2) no
C23 C214 C215 C216 3.6(4) no
C213 C214 C215 C232 -1.0(3) no
C23 C214 C215 C232 140.9(2) no
C214 C215 C216 C217 -0.6(4) no
C214 C215 C232 C231 1.0(3) no
C214 C215 C232 C233 -141.1(2) no
C214 C215 C216 C234 141.5(2) no
C216 C215 C232 C233 0.3(3) no
C232 C215 C216 C234 -0.3(3) no
C232 C215 C216 C217 -142.3(2) no
C216 C215 C232 C231 142.4(2) no
C215 C216 C217 C24 -1.5(4) no
C234 C216 C217 C218 1.3(4) no
C215 C216 C234 C233 0.2(3) no
C215 C216 C217 C218 138.5(2) no
C217 C216 C234 C235 -1.6(4) no
C215 C216 C234 C235 -143.3(2) no
C234 C216 C217 C24 -138.7(3) no
C217 C216 C234 C233 141.8(2) no
C216 C217 C218 C236 -0.3(4) no
C24 C217 C218 C236 144.1(2) no
C216 C217 C218 C219 -143.7(2) no
C24 C217 C218 C219 0.8(3) no
C217 C218 C219 C25 -1.0(3) no
C219 C218 C236 C237 0.8(4) no
C217 C218 C219 C220 144.0(2) no
C217 C218 C236 C237 -138.3(3) no
C236 C218 C219 C220 0.4(4) no

C219 C218 C236 C235 138.8(2) no
C236 C218 C219 C25 -144.6(2) no
C217 C218 C236 C235 -0.4(4) no
C218 C219 C220 C221 -137.7(2) no
C218 C219 C220 C238 -1.5(4) no
C25 C219 C220 C221 2.7(4) no
C25 C219 C220 C238 138.9(2) no
C221 C220 C238 C239 -0.1(3) no
C219 C220 C221 C27 -0.8(3) no
C219 C220 C238 C239 -141.0(2) no
C238 C220 C221 C27 -142.2(2) no
C221 C220 C238 C237 142.3(2) no
C219 C220 C238 C237 1.4(4) no
C219 C220 C221 C222 141.5(2) no
C238 C220 C221 C222 0.1(3) no
C27 C221 C222 C223 -0.4(3) no
C27 C221 C222 C239 141.9(2) no
C220 C221 C222 C223 -142.5(2) no
C220 C221 C222 C239 -0.1(3) no
C221 C222 C223 C224 0.0(3) no
C223 C222 C239 C240 0.0(3) no
C221 C222 C223 C242 137.9(2) no
C239 C222 C223 C224 -137.9(2) no
C239 C222 C223 C242 0.0(4) no
C221 C222 C239 C238 0.1(3) no
C221 C222 C239 C240 -142.8(2) no
C223 C222 C239 C238 143.0(2) no
C222 C223 C224 C28 0.4(3) no
C222 C223 C224 C225 143.0(2) no
C242 C223 C224 C28 -142.4(2) no
C242 C223 C224 C225 0.2(3) no
C222 C223 C242 C241 -0.1(4) no
C222 C223 C242 C243 -142.0(2) no
C224 C223 C242 C241 142.2(2) no
C224 C223 C242 C243 0.2(3) no
C223 C224 C225 C243 -0.5(3) no
C223 C224 C225 C226 -142.4(2) no
C28 C224 C225 C226 0.4(4) no
C28 C224 C225 C243 142.3(2) no
C224 C225 C226 C227 137.7(2) no
C224 C225 C243 C242 0.6(3) no
C243 C225 C226 C210 -138.5(2) no
C243 C225 C226 C227 0.7(4) no
C224 C225 C226 C210 -1.5(4) no
C226 C225 C243 C244 -0.5(4) no
C224 C225 C243 C244 -141.9(2) no
C226 C225 C243 C242 142.0(2) no
C210 C226 C227 C228 0.0(3) no
C210 C226 C227 C245 143.4(2) no
C225 C226 C227 C228 -143.6(2) no
C225 C226 C227 C245 -0.2(4) no
C245 C227 C228 C229 0.9(4) no
C226 C227 C245 C244 -0.4(4) no
C226 C227 C245 C246 -139.0(2) no
C228 C227 C245 C244 138.4(2) no
C228 C227 C245 C246 -0.2(4) no
C226 C227 C228 C211 -0.3(3) no
C226 C227 C228 C229 144.0(2) no
C245 C227 C228 C211 -143.4(2) no
C227 C228 C229 C247 -1.0(4) no
C211 C228 C229 C230 1.6(4) no
C211 C228 C229 C247 139.0(2) no
C227 C228 C229 C230 -138.4(2) no
C228 C229 C230 C213 0.2(4) no
C228 C229 C230 C231 142.2(2) no
C247 C229 C230 C213 -141.7(2) no
C230 C229 C247 C246 142.3(2) no

C230 C229 C247 C248 -0.3(3) no
C228 C229 C247 C248 -142.0(2) no
C247 C229 C230 C231 0.3(3) no
C228 C229 C247 C246 0.6(4) no
C213 C230 C231 C248 141.4(2) no
C213 C230 C231 C232 -0.8(3) no
C229 C230 C231 C232 -142.3(2) no
C229 C230 C231 C248 -0.2(3) no
C230 C231 C232 C215 -0.2(3) no
C230 C231 C248 C247 0.0(3) no
C230 C231 C248 C249 -142.2(2) no
C232 C231 C248 C247 141.9(2) no
C232 C231 C248 C249 -0.2(3) no
C230 C231 C232 C233 137.6(2) no
C248 C231 C232 C215 -137.7(2) no
C248 C231 C232 C233 0.0(3) no
C131 C31 C32 C33 178.4(4) no
C36 C31 C32 C33 -0.1(8) no
C32 C31 C36 C35 0.1(8) no
C131 C31 C36 C35 -178.4(4) no
C31 C32 C33 C34 0.1(8) no
C215 C232 C233 C234 -0.2(3) no
C231 C232 C233 C250 0.3(3) no
C231 C232 C233 C234 -142.4(2) no
C215 C232 C233 C250 142.6(2) no
C232 C233 C234 C235 143.5(2) no
C232 C233 C250 C249 -0.5(3) no
C232 C233 C234 C216 0.0(3) no
C234 C233 C250 C251 -0.1(4) no
C250 C233 C234 C216 -142.9(2) no
C250 C233 C234 C235 0.6(4) no
C234 C233 C250 C249 137.7(2) no
C32 C33 C34 C35 -0.1(8) no
C232 C233 C250 C251 -138.3(2) no
C216 C234 C235 C236 0.9(4) no
C33 C34 C35 C36 0.1(8) no
C233 C234 C235 C252 -0.7(4) no
C216 C234 C235 C252 138.6(3) no
C233 C234 C235 C236 -138.4(2) no
C234 C235 C252 C251 0.3(4) no
C252 C235 C236 C237 0.2(3) no
C234 C235 C252 C253 -142.1(2) no
C252 C235 C236 C218 -142.1(2) no
C236 C235 C252 C253 0.1(3) no
C234 C235 C236 C237 142.4(2) no
C236 C235 C252 C251 142.5(2) no
C234 C235 C236 C218 0.1(4) no
C34 C35 C36 C31 0.0(8) no
C218 C236 C237 C238 -0.9(4) no
C218 C236 C237 C253 141.6(2) no
C235 C236 C237 C238 -143.0(2) no
C235 C236 C237 C253 -0.5(3) no
C238 C237 C253 C254 0.0(4) no
C238 C237 C253 C252 143.2(2) no
C236 C237 C238 C220 -0.2(4) no
C236 C237 C253 C252 0.5(3) no
C236 C237 C253 C254 -142.6(2) no
C236 C237 C238 C239 137.8(2) no
C253 C237 C238 C220 -138.3(2) no
C253 C237 C238 C239 -0.4(4) no
C220 C238 C239 C240 142.8(2) no
C237 C238 C239 C222 -142.3(2) no
C237 C238 C239 C240 0.6(4) no
C220 C238 C239 C222 0.0(3) no
C238 C239 C240 C254 -0.5(4) no
C222 C239 C240 C241 0.0(4) no
C238 C239 C240 C241 -138.5(2) no

C222	C239	C240	C254	138.1(2)	.	.	.	.	no
C239	C240	C241	C242	-0.1(4)	.	.	.	.	no
C239	C240	C241	C260	142.1(2)	.	.	.	.	no
C239	C240	C254	C255	-142.6(2)	.	.	.	.	no
C241	C240	C254	C253	142.6(2)	.	.	.	.	no
C241	C240	C254	C255	-0.2(3)	.	.	.	.	no
C239	C240	C254	C253	0.1(4)	.	.	.	.	no
C254	C240	C241	C242	-142.3(2)	.	.	.	.	no
C254	C240	C241	C260	-0.2(3)	.	.	.	.	no
C260	C241	C242	C223	-137.8(2)	.	.	.	.	no
C240	C241	C260	C259	-142.3(2)	.	.	.	.	no
C260	C241	C242	C243	-0.5(4)	.	.	.	.	no
C240	C241	C260	C255	0.4(3)	.	.	.	.	no
C240	C241	C242	C243	137.4(2)	.	.	.	.	no
C240	C241	C242	C223	0.1(4)	.	.	.	.	no
C242	C241	C260	C255	142.9(2)	.	.	.	.	no
C242	C241	C260	C259	0.2(4)	.	.	.	.	no
C241	C242	C243	C225	-142.1(2)	.	.	.	.	no
C223	C242	C243	C225	-0.5(3)	.	.	.	.	no
C223	C242	C243	C244	141.8(2)	.	.	.	.	no
C241	C242	C243	C244	0.2(4)	.	.	.	.	no
C242	C243	C244	C245	-138.2(2)	.	.	.	.	no
C225	C243	C244	C259	138.4(2)	.	.	.	.	no
C242	C243	C244	C259	0.3(4)	.	.	.	.	no
C225	C243	C244	C245	-0.1(4)	.	.	.	.	no
C243	C244	C245	C246	143.3(2)	.	.	.	.	no
C259	C244	C245	C227	-142.5(2)	.	.	.	.	no
C259	C244	C245	C246	0.3(3)	.	.	.	.	no
C243	C244	C259	C258	-142.9(2)	.	.	.	.	no
C243	C244	C245	C227	0.5(4)	.	.	.	.	no
C243	C244	C259	C260	-0.6(4)	.	.	.	.	no
C245	C244	C259	C258	0.1(3)	.	.	.	.	no
C245	C244	C259	C260	142.4(2)	.	.	.	.	no
C227	C245	C246	C247	-0.3(4)	.	.	.	.	no
C227	C245	C246	C258	142.3(2)	.	.	.	.	no
C244	C245	C246	C247	-143.3(2)	.	.	.	.	no
C244	C245	C246	C258	-0.6(3)	.	.	.	.	no
C245	C246	C258	C257	-142.6(2)	.	.	.	.	no
C245	C246	C258	C259	0.7(3)	.	.	.	.	no
C258	C246	C247	C229	-138.2(2)	.	.	.	.	no
C247	C246	C258	C259	143.5(2)	.	.	.	.	no
C258	C246	C247	C248	-0.4(4)	.	.	.	.	no
C247	C246	C258	C257	0.2(4)	.	.	.	.	no
C245	C246	C247	C229	0.1(4)	.	.	.	.	no
C245	C246	C247	C248	138.0(2)	.	.	.	.	no
C229	C247	C248	C231	0.2(3)	.	.	.	.	no
C229	C247	C248	C249	142.7(2)	.	.	.	.	no
C246	C247	C248	C231	-142.2(2)	.	.	.	.	no
C246	C247	C248	C249	0.3(4)	.	.	.	.	no
C247	C248	C249	C250	-137.9(2)	.	.	.	.	no
C247	C248	C249	C257	-0.2(3)	.	.	.	.	no
C231	C248	C249	C257	137.8(2)	.	.	.	.	no
C231	C248	C249	C250	0.1(3)	.	.	.	.	no
C248	C249	C257	C258	0.1(4)	.	.	.	.	no
C248	C249	C250	C233	0.3(3)	.	.	.	.	no
C248	C249	C257	C256	-142.2(2)	.	.	.	.	no
C250	C249	C257	C258	142.2(2)	.	.	.	.	no
C248	C249	C250	C251	142.5(2)	.	.	.	.	no
C250	C249	C257	C256	0.0(3)	.	.	.	.	no
C257	C249	C250	C251	0.1(3)	.	.	.	.	no
C257	C249	C250	C233	-142.2(2)	.	.	.	.	no
C249	C250	C251	C256	-0.1(3)	.	.	.	.	no
C233	C250	C251	C252	-0.3(4)	.	.	.	.	no
C249	C250	C251	C252	-142.6(2)	.	.	.	.	no
C233	C250	C251	C256	142.2(2)	.	.	.	.	no
C250	C251	C252	C235	0.3(4)	.	.	.	.	no
C250	C251	C252	C253	138.4(2)	.	.	.	.	no

C250	C251	C256	C257	0.1(3)		no
C252	C251	C256	C255	-0.4(4)		no
C252	C251	C256	C257	142.5(2)		no
C250	C251	C256	C255	-142.8(2)		no
C256	C251	C252	C235	-137.8(2)		no
C256	C251	C252	C253	0.3(4)		no
C235	C252	C253	C254	142.7(2)		no
C251	C252	C253	C237	-143.1(2)		no
C251	C252	C253	C254	0.0(4)		no
C235	C252	C253	C237	-0.4(3)		no
C237	C253	C254	C240	0.1(4)		no
C237	C253	C254	C255	138.5(2)		no
C252	C253	C254	C240	-138.5(2)		no
C252	C253	C254	C255	-0.2(4)		no
C253	C254	C255	C260	-142.5(2)		no
C240	C254	C255	C256	143.0(2)		no
C240	C254	C255	C260	0.4(3)		no
C253	C254	C255	C256	0.1(4)		no
C254	C255	C260	C241	-0.5(3)		no
C260	C255	C256	C251	138.4(2)		no
C254	C255	C256	C257	-138.0(3)		no
C256	C255	C260	C259	-0.5(4)		no
C254	C255	C260	C259	142.3(2)		no
C256	C255	C260	C241	-143.3(2)		no
C254	C255	C256	C251	0.2(4)		no
C260	C255	C256	C257	0.3(4)		no
C255	C256	C257	C258	0.6(4)		no
C251	C256	C257	C258	-142.1(2)		no
C255	C256	C257	C249	142.7(2)		no
C251	C256	C257	C249	0.0(3)		no
C249	C257	C258	C246	-0.1(3)		no
C249	C257	C258	C259	-139.2(2)		no
C256	C257	C258	C259	-1.2(4)		no
C256	C257	C258	C246	137.9(2)		no
C257	C258	C259	C244	143.2(2)		no
C257	C258	C259	C260	1.0(4)		no
C246	C258	C259	C260	-142.6(2)		no
C246	C258	C259	C244	-0.5(3)		no
C244	C259	C260	C255	-137.9(2)		no
C258	C259	C260	C241	138.0(2)		no
C258	C259	C260	C255	-0.2(4)		no
C244	C259	C260	C241	0.3(4)		no
C262	C261	C268	C269	-76.6(3)		no
C21	C261	C262	C267	126.3(3)		no
C22	C261	C262	C267	52.6(3)		no
C21	C261	C262	C263	-56.4(3)		no
C21	C261	C268	C269	68.6(3)		no
C22	C261	C262	C263	-130.0(3)		no
C22	C261	C268	C269	142.2(2)		no
C268	C261	C262	C263	87.7(3)		no
C268	C261	C262	C267	-89.6(3)		no
C263	C262	C267	C266	0.4(4)		no
C261	C262	C267	C266	177.8(2)		no
C261	C262	C263	C264	-176.8(3)		no
C267	C262	C263	C264	0.5(4)		no
C262	C263	C264	C265	-1.1(4)		no
C263	C264	C265	C266	0.8(4)		no
C264	C265	C266	C267	0.2(4)		no
C265	C266	C267	C262	-0.7(4)		no
C261	C268	C269	C270	-173.6(2)		no
C268	C269	C270	C271	76.6(3)		no
C269	C270	C271	O21	108.5(3)		no
C269	C270	C271	O22	-70.8(3)		no
C141	C41	C42	C43	-179.7(2)		no
C46	C41	C42	C43	-0.1(5)		no
C141	C41	C46	C45	179.8(2)		no
C42	C41	C46	C45	0.1(5)		no

C41	C42	C43	C44	0.07	.	.	.	.	no
C42	C43	C44	C45	-0.07	.	.	.	.	no
C43	C44	C45	C46	0.08	.	.	.	.	no
C44	C45	C46	C41	-0.08	.	.	.	.	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									
C131	C136	3.577(3)	.	1_455	no				
C131	C231	3.631(3)	.	1_545	no				
C141	C125	3.413(3)	.	.	no				
C141	C141	3.469(3)	.	2_666	no				
C141	C126	3.604(3)	.	.	no				
C141	C221	3.588(3)	.	.	no				
C141	C124	3.484(3)	.	.	no				
C141	C27	3.644(3)	.	.	no				
C131	H170	3.0961	.	.	no				
O11	C42	3.171(4)	.	.	no				
O11	C28	3.207(3)	.	.	no				
O11	C139	3.353(3)	.	1_455	no				
O11	C43	3.336(4)	.	.	no				
O11	C138	3.361(3)	.	1_455	no				
O11	C46	3.162(4)	.	2_566	no				
O11	C45	3.352(4)	.	2_566	no				
O12	C32	3.299(6)	.	.	no				
O12	C35	3.235(6)	.	2_565	no				
O12	C34	3.282(5)	.	2_565	no				
O12	C224	3.362(3)	.	.	no				
O12	C31	3.248(5)	.	.	no				
O21	C172	3.094(4)	.	.	no				
O21	C237	3.282(3)	.	1_455	no				
O21	C253	3.278(3)	.	1_455	no				
O22	C268	3.051(4)	.	.	no				
O11	H172	2.4505	.	.	no				
O11	H42	2.4606	.	.	no				
O11	H45	2.8363	.	2_566	no				
O11	H172"	2.7629	.	.	no				
O11	H269'	2.7866	.	.	no				
O11	H46	2.4446	.	2_566	no				
O11	H43	2.8027	.	.	no				
O12	H169'	2.7274	.	.	no				
O21	H272"	2.6053	.	.	no				
O21	H172	2.8902	.	.	no				
O21	H272	2.6394	.	.	no				
O21	H172"	2.4061	.	.	no				
O22	H268'	2.3518	.	.	no				
C13	C163	3.444(4)	.	.	no				
C14	C162	3.429(4)	.	.	no				
C14	C260	3.574(3)	.	2_665	no				
C15	C162	3.457(4)	.	.	no				
C15	C167	3.441(4)	.	.	no				
C16	C167	3.144(3)	.	.	no				
C17	C238	3.331(3)	.	.	no				
C17	C239	3.204(3)	.	.	no				
C18	C220	3.499(3)	.	.	no				
C18	C238	3.594(3)	.	.	no				
C18	C221	3.579(3)	.	.	no				
C19	C169	3.598(4)	.	.	no				
C23	C267	3.147(4)	.	.	no				
C24	C262	3.396(4)	.	.	no				
C25	C262	3.434(4)	.	.	no				
C26	C263	3.309(4)	.	.	no				
C27	C141	3.644(3)	.	.	no				

C27 C45 3.429(4) . 2_566 no
C28 C171 3.419(4) . . no
C28 O11 3.207(3) . . no
C29 C269 3.393(4) . . no
C31 O12 3.248(5) . . no
C31 C172 3.577(6) . 2_565 no
C32 O12 3.299(6) . . no
C32 C172 3.592(6) . 2_565 no
C34 O12 3.282(5) . 2_565 no
C35 O12 3.235(6) . 2_565 no
C42 C263 3.546(4) . . no
C42 O11 3.171(4) . . no
C43 C140 3.521(4) . 1_455 no
C43 O11 3.336(4) . . no
C45 O11 3.352(4) . 2_566 no
C45 C27 3.429(4) . 2_566 no
C46 C264 3.576(4) . . no
C46 O11 3.162(4) . 2_566 no
C110 C168 3.419(4) . . no
C111 C168 3.419(4) . . no
C11 H167 2.8674 . . no
C11 H169 3.0432 . . no
C12 H163 3.0905 . . no
C112 C234 3.560(3) . 1_545 no
C112 C233 3.529(3) . 1_545 no
C113 C234 2.943(3) . 1_545 no
C113 C233 3.287(4) . 1_545 no
C113 C235 3.559(3) . 1_545 no
C114 C233 3.547(4) . 1_545 no
C114 C234 3.547(4) . 1_545 no
C15 H166 2.8325 . 2_665 no
C16 H167 2.6696 . . no
C116 C244 3.599(3) . 2_665 no
C116 C259 3.352(3) . 2_665 no
C117 C244 3.478(3) . 2_665 no
C117 C259 3.313(3) . 2_665 no
C19 H168 2.7636 . . no
C19 H169 3.0422 . . no
C21 H269' 2.8485 . . no
C21 H263 3.0206 . . no
C22 H267 2.8139 . . no
C23 H266 2.9716 . 2_576 no
C123 C143 3.380(3) . 2_666 no
C123 C142 3.474(4) . 2_666 no
C23 H267 2.8134 . . no
C124 C141 3.484(3) . . no
C125 C141 3.413(3) . . no
C126 C141 3.604(3) . . no
C26 H263 3.0490 . . no
C27 H45 2.7569 . 2_566 no
C28 H172 2.8958 . . no
C129 C147 3.446(3) . 2_656 no
C29 H269' 2.7705 . . no
C29 H172 2.8214 . . no
C29 H268' 2.8730 . . no
C130 C234 3.393(4) . 1_545 no
C31 H172' 2.6122 . 2_565 no
C32 H172' 2.7838 . 2_565 no
C133 C268 3.577(4) . 1_645 no
C133 C212 3.238(3) . 1_645 no
C33 H172' 3.0912 . . no
C34 H172' 2.7132 . . no
C134 C212 3.546(3) . 1_645 no
C134 C213 3.525(4) . 1_645 no
C135 C230 3.588(4) . 1_645 no
C135 C213 3.496(3) . 1_645 no
C35 H169' 3.0158 . 2_565 no

C35 H172' 2.7639 . . no
C36 H172' 3.0600 . 2_565 no
C136 C131 3.577(3) . 1_655 no
C137 C170 3.355(4) . 1_655 no
C137 C171 3.211(4) . 1_655 no
C138 O11 3.361(3) . 1_655 no
C138 C171 3.330(4) . 1_655 no
C138 C172 3.528(4) . 1_655 no
C139 O11 3.353(3) . 1_655 no
C140 C43 3.521(4) . 1_655 no
C141 C141 3.469(3) . 2_666 no
C41 H263 2.9293 . . no
C142 C142 3.142(4) . 2_666 no
C142 C123 3.474(4) . 2_666 no
C42 H264 3.0273 . 2_566 no
C142 C143 3.244(3) . 2_666 no
C42 H263 2.6465 . . no
C143 C142 3.244(3) . 2_666 no
C43 H263 2.8589 . . no
C143 C123 3.380(3) . 2_666 no
C145 C270 3.434(4) . 2_566 no
C45 H264 2.8281 . . no
C46 H264 2.8498 . . no
C46 H263 2.9158 . 2_566 no
C146 C147 3.558(3) . 2_656 no
C147 C129 3.446(3) . 2_656 no
C147 C147 2.902(3) . 2_656 no
C147 C146 3.558(3) . 2_656 no
C147 C148 3.410(3) . 2_656 no
C148 C147 3.410(3) . 2_656 no
C150 C212 3.506(3) . 1_645 no
C152 C213 3.584(3) . 1_645 no
C153 C171 3.582(4) . 1_655 no
C153 C170 3.304(4) . 1_655 no
C158 C218 3.341(3) . 2_666 no
C158 C217 3.530(3) . 2_666 no
C159 C219 3.407(4) . 2_666 no
C159 C218 3.187(4) . 2_666 no
C160 C219 3.480(3) . 2_666 no
C162 C15 3.457(4) . . no
C162 C14 3.429(4) . . no
C163 C13 3.444(4) . . no
C164 C254 3.271(4) . 2_665 no
C165 C254 3.533(4) . 2_665 no
C165 C240 3.381(4) . 2_665 no
C167 C15 3.441(4) . . no
C167 C169 3.581(4) . . no
C167 C16 3.144(3) . . no
C168 C110 3.419(4) . . no
C168 C111 3.419(4) . . no
C169 C167 3.581(4) . . no
C169 C19 3.598(4) . . no
C170 C137 3.355(4) . 1_455 no
C170 C153 3.304(4) . 1_455 no
C171 C224 3.572(4) . . no
C171 C153 3.582(4) . 1_455 no
C171 C138 3.330(4) . 1_455 no
C171 C137 3.211(4) . 1_455 no
C171 C28 3.419(4) . . no
C172 C225 3.572(4) . . no
C172 O21 3.094(4) . . no
C172 C138 3.528(4) . 1_455 no
C172 C224 3.513(4) . . no
C172 C31 3.577(6) . 2_565 no
C172 C32 3.592(6) . 2_565 no
C210 C272 3.511(5) . . no
C210 C268 3.408(4) . . no

C110 H168 2.7208 . . no
C211 C268 3.441(4) . . no
C111 H168 2.6832 . . no
C212 C134 3.546(3) . 1_465 no
C212 C133 3.238(3) . 1_465 no
C112 H168 2.6893 . . no
C212 C150 3.506(3) . 1_465 no
C213 C134 3.525(4) . 1_465 no
C213 C135 3.496(3) . 1_465 no
C213 C152 3.584(3) . 1_465 no
C217 C158 3.530(3) . 2_666 no
C118 H33 3.0737 . 2_665 no
C218 C159 3.187(4) . 2_666 no
C218 C158 3.341(3) . 2_666 no
C119 H165 2.9735 . 2_665 no
C219 C160 3.480(3) . 2_666 no
C219 C159 3.407(4) . 2_666 no
C119 H166 2.9673 . 2_665 no
C120 H172" 3.0621 . 1_655 no
C120 H165 2.8560 . 2_665 no
C220 C18 3.499(3) . . no
C221 C18 3.579(3) . . no
C221 C141 3.588(3) . . no
C224 O12 3.362(3) . . no
C224 C171 3.572(4) . . no
C224 C172 3.513(4) . . no
C225 C172 3.572(4) . . no
C227 C247 3.494(4) . 2_575 no
C227 C246 3.509(4) . 2_575 no
C127 H269 2.9846 . 2_566 no
C228 C245 3.411(3) . 2_575 no
C228 C246 3.513(4) . 2_575 no
C229 C245 3.484(3) . 2_575 no
C230 C135 3.588(4) . 1_465 no
C231 C131 3.631(3) . 1_565 no
C133 H268' 3.0929 . 1_645 no
C233 C114 3.547(4) . 1_565 no
C233 C112 3.529(3) . 1_565 no
C233 C113 3.287(4) . 1_565 no
C234 C112 3.560(3) . 1_565 no
C234 C114 3.547(4) . 1_565 no
C234 C113 2.943(3) . 1_565 no
C234 C130 3.393(4) . 1_565 no
C235 C113 3.559(3) . 1_565 no
C237 C271 3.477(4) . 1_655 no
C237 O21 3.282(3) . 1_655 no
C137 H170 2.8627 . 1_655 no
C238 C17 3.331(3) . . no
C138 H172" 2.7811 . 1_655 no
C238 C18 3.594(3) . . no
C239 C17 3.204(3) . . no
C140 H43 2.6947 . 1_655 no
C240 C165 3.381(4) . 2_665 no
C244 C116 3.599(3) . 2_665 no
C244 C117 3.478(3) . 2_665 no
C245 C229 3.484(3) . 2_575 no
C145 H270 2.9081 . 2_566 no
C245 C228 3.411(3) . 2_575 no
C246 C228 3.513(4) . 2_575 no
C246 C227 3.509(4) . 2_575 no
C247 C227 3.494(4) . 2_575 no
C148 H268 3.0056 . 1_645 no
C149 H268 2.9485 . 1_645 no
C149 H267 2.9985 . 1_645 no
C150 H268 3.0256 . 1_645 no
C150 H267 2.9210 . 1_645 no
C251 C257 3.562(4) . 2_675 no

C251 C256 3.431(3) . 2_675 no
C153 H170 2.9436 . 1_655 no
C153 H170' 3.0354 . 1_655 no
C253 C271 3.534(4) . 1_655 no
C253 O21 3.278(3) . 1_655 no
C254 C164 3.271(4) . 2_665 no
C254 C165 3.533(4) . 2_665 no
C256 C257 3.551(4) . 2_675 no
C256 C251 3.431(3) . 2_675 no
C256 C256 3.227(4) . 2_675 no
C257 C256 3.551(4) . 2_675 no
C257 C251 3.562(4) . 2_675 no
C258 C272 3.550(5) . 2_575 no
C259 C117 3.313(3) . 2_665 no
C259 C116 3.352(3) . 2_665 no
C260 C14 3.574(3) . 2_665 no
C162 H169' 2.8028 . . no
C262 C25 3.434(4) . . no
C262 C24 3.396(4) . . no
C263 C269 3.497(4) . . no
C263 C26 3.309(4) . . no
C163 H168' 2.8375 . . no
C263 C42 3.546(4) . . no
C163 H35 2.9986 . 2_565 no
C164 H35 2.8868 . 2_565 no
C264 C46 3.576(4) . . no
C164 H32 2.9996 . . no
C165 H35 2.9747 . 2_565 no
C165 H32 2.9169 . . no
C166 H32 3.0176 . . no
C167 H169' 3.0138 . . no
C267 C23 3.147(4) . . no
C268 C210 3.408(4) . . no
C168 H163 3.0965 . . no
C268 O22 3.051(4) . . no
C268 C133 3.577(3) . 1_465 no
C268 C211 3.441(4) . . no
C269 C29 3.393(4) . . no
C269 C263 3.497(4) . . no
C270 C145 3.434(4) . 2_566 no
C271 C253 3.534(4) . 1_455 no
C271 C237 3.477(4) . 1_455 no
C272 C258 3.550(5) . 2_575 no
C272 C210 3.511(5) . . no
C210 H268' 2.7877 . . no
C210 H172 2.9491 . . no
C210 H272" 3.0702 . . no
C211 H268' 2.6741 . . no
C212 H268' 2.6535 . . no
C214 H266 2.9080 . 2_576 no
C215 H266 2.9860 . 2_576 no
C215 H265 3.0550 . 2_576 no
C222 H169 3.0461 . . no
C222 H167 2.9277 . . no
C223 H167 2.9053 . . no
C224 H172 3.0415 . . no
C226 H272" 3.0997 . . no
C233 H163 3.0271 . 1_565 no
C243 H33 3.0846 . . no
C246 H272' 2.8243 . 2_575 no
C248 H163 3.0631 . 1_565 no
C249 H163 2.9343 . 1_565 no
C250 H163 2.9126 . 1_565 no
C252 H272 2.8888 . 1_655 no
C253 H272 2.7929 . 1_655 no
C254 H164 2.9084 . 2_665 no
C258 H272' 2.7553 . 2_575 no

C262 H269 2.9607 . . no
C263 H269 2.8945 . . no
C267 H268 3.0738 . . no
C271 H268' 2.9050 . . no
H168' H170 2.3288 . . no
H168' H163 2.5860 . . no
H168' C163 2.8375 . . no
H169' C35 3.0158 . 2_565 no
H169' H35 2.5473 . 2_565 no
H169' C167 3.0138 . . no
H169' C162 2.8028 . . no
H169' O12 2.7274 . . no
H170' H168 2.5042 . . no
H170' H264 2.4721 . 2_566 no
H170' C153 3.0354 . 1_455 no
H172' C34 2.7132 . . no
H172' C35 2.7639 . . no
H172' C33 3.0912 . . no
H172' C36 3.0600 . 2_565 no
H172' C32 2.7838 . 2_565 no
H172' C31 2.6122 . 2_565 no
H172" O21 2.4061 . . no
H172" C138 2.7811 . 1_455 no
H172" O11 2.7629 . . no
H172" C120 3.0621 . 1_455 no
H268' C133 3.0929 . 1_465 no
H268' C29 2.8730 . . no
H268' C271 2.9050 . . no
H268' C210 2.7877 . . no
H268' C211 2.6741 . . no
H268' C212 2.6535 . . no
H268' O22 2.3518 . . no
H269' O11 2.7866 . . no
H269' C29 2.7705 . . no
H269' C21 2.8485 . . no
H272' C246 2.8243 . 2_575 no
H272' C258 2.7553 . 2_575 no
H272" C210 3.0702 . . no
H272" C226 3.0997 . . no
H272" O21 2.6053 . . no
H32 C165 2.9169 . . no
H32 C166 3.0176 . . no
H32 C164 2.9996 . . no
H33 C118 3.0737 . 2_665 no
H33 C243 3.0846 . . no
H35 C163 2.9986 . 2_565 no
H35 C165 2.9747 . 2_565 no
H35 H169' 2.5473 . 2_565 no
H35 C164 2.8868 . 2_565 no
H42 O11 2.4606 . . no
H43 C140 2.6947 . 1_455 no
H43 O11 2.8027 . . no
H45 O11 2.8363 . 2_566 no
H45 C27 2.7569 . 2_566 no
H46 O11 2.4446 . 2_566 no
H163 C12 3.0905 . . no
H163 C250 2.9126 . 1_545 no
H163 H168' 2.5860 . . no
H163 C248 3.0631 . 1_545 no
H163 C168 3.0965 . . no
H163 C233 3.0271 . 1_545 no
H163 C249 2.9343 . 1_545 no
H164 C254 2.9084 . 2_665 no
H165 C119 2.9735 . 2_665 no
H165 C120 2.8560 . 2_665 no
H166 C15 2.8325 . 2_665 no
H166 C119 2.9673 . 2_665 no

H167 C222 2.9277 . . no
H167 C16 2.6696 . . no
H167 C223 2.9053 . . no
H167 C11 2.8674 . . no
H168 C112 2.6893 . . no
H168 C111 2.6832 . . no
H168 C110 2.7208 . . no
H168 H170' 2.5042 . . no
H168 C19 2.7636 . . no
H169 C19 3.0422 . . no
H169 C222 3.0461 . . no
H169 C11 3.0432 . . no
H170 C131 3.0961 . . no
H170 C153 2.9436 . 1_455 no
H170 H168' 2.3288 . . no
H170 C137 2.8627 . 1_455 no
H172 O21 2.8902 . . no
H172 C210 2.9491 . . no
H172 C28 2.8958 . . no
H172 C29 2.8214 . . no
H172 C224 3.0415 . . no
H172 O11 2.4505 . . no
H263 C21 3.0206 . . no
H263 H269 2.5929 . . no
H263 C46 2.9158 . 2_566 no
H263 C41 2.9293 . . no
H263 C42 2.6465 . . no
H263 C26 3.0490 . . no
H263 C43 2.8589 . . no
H264 C45 2.8281 . . no
H264 C46 2.8498 . . no
H264 C42 3.0273 . 2_566 no
H264 H170' 2.4721 . 2_566 no
H265 C215 3.0550 . 2_576 no
H266 C214 2.9080 . 2_576 no
H266 C215 2.9860 . 2_576 no
H266 C23 2.9716 . 2_576 no
H267 C22 2.8139 . . no
H267 C150 2.9210 . 1_465 no
H267 C23 2.8134 . . no
H267 C149 2.9985 . 1_465 no
H268 C267 3.0738 . . no
H268 H270 2.5817 . . no
H268 C150 3.0256 . 1_465 no
H268 C148 3.0056 . 1_465 no
H268 C149 2.9485 . 1_465 no
H269 C263 2.8945 . . no
H269 C262 2.9607 . . no
H269 H263 2.5929 . . no
H269 C127 2.9846 . 2_566 no
H270 H268 2.5817 . . no
H270 C145 2.9081 . 2_566 no
H272 C253 2.7929 . 1_455 no
H272 O21 2.6394 . . no
H272 C252 2.8888 . 1_455 no

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)
#
C172 H172" O21 1.0000 2.4100 3.094(4) 125.00 . yes
C268 H268' O22 1.0200 2.3500 3.051(4) 125.00 . yes
C42  H42  O11 0.9500 2.4600 3.171(4) 132.00 . yes
C46  H46  O11 0.9500 2.4400 3.162(4) 132.00 2_566 yes

#===END of Crystallographic Information File
```