Low-valent pentafulvene titanium dinitrogen complex as a precursor for cationic titanium complexes

Scherer, Axel; Haase, Detlev; Saak, Wolfgang; Beckhaus, Ruediger; Meetsma, Auke; Bouwkamp, Marco W.; Beckhaus, Rüdiger

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2009

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# CIF-file generated for C64H83BO3Ti                              CP870
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2009-09-28 # Formatted by publCIF
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# 1. SUBMISSION DETAILS

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

_publ_requested_journal              'Organometallics'
# Publication choise FI FM FO CI CM CO
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2009-09-28  11:45:40

 Consider this CIF submission for deposition of the first
 X-ray structure of a manuscript to be submitted to : Organometallics.
  (Our Compound_Identification_Code : CP870)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_printers_final         ?
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_journal_page_last                   ?


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# 3. TITLE AND AUTHOR LIST

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Title (type here to add)
;
_publ_section_title_footnote
.

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


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
 Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
```

```
  NL-9747 AG Groningen, The Netherlands.
;

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

# 4. TEXT

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;

# Insert blank lines between paragraphs

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;
_publ_section_exptl_prep
;
(type here to add preparation details)
;
_publ_section_exptl_refinement
;
Some atoms of the solvent molecules showed unrealistic displacement parameters
when allowed to vary anisotropically, suggesting dynamic disorder (dynamic
means that the smeared electron density is due to fluctuations of the atomic
positions within each unit cell).
;

# Insert blank lines between references

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Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S. Gould, R.O.
Isra\"el, R. & Smits, J.M.M.  (1999). The <i>DIRDIF99</i> program system,
Technical Report of the Crystallography Laboratory, University of Nijmegen,
The Netherlands.

Bruker,      (2001). <i>SMART</i>, <i>SAINT</i>, <i>SADABS</i>, <i>XPREP</i>
and <i>SHELXTL</i>/NT. Software Reference Manual Bruker AXS Inc. Madison,
Wisconsin, USA.

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

Meetsma, A. (2003). Extended version of the program <i>PLUTO</i>. Groningen
University, The Netherlands. (unpublished).

Sheldrick, G.M. <i>SHELXL97</i>. Program for Crystal Structure Refinement.
University of G\"ottingen, Germany, 1997.

Spek, A. L. (2003). <i>J. Appl. Cryst.</i> <b>36</b>, 7--13.

;


_publ_section_figure_captions
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;
Fig. 1. Perspective <i>PLUTO</i> drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective <i>ORTEP</i> drawing of the title compound. Displacement
ellipsoids for non-H are represented at the 50% probability level. The H-atoms
have been omitted to improve clarity.
;

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# 5. CHEMICAL DATA

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; ?
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
'C29 H41 O Ti, C24 H20 B, 0.5(C6 H12), 2(C4 H8 O)'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural          ?
_chemical_formula_sum
'C64 H83 B O3 Ti'
_chemical_formula_iupac               ?
_chemical_formula_weight                 958.98
_chemical_compound_source            'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Ti  Ti    0.2776    0.4457
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 O   O    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 B   B    0.0013    0.0007
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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# 6. CRYSTAL DATA

_symmetry_cell_setting                Monoclinic
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_symmetry_space_group_name_H-M       'P 21/n'
_symmetry_Int_Tables_number                14

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                          11.7758(8)
_cell_length_b                          22.193(2)
_cell_length_c                          21.726(2)
_cell_angle_alpha                       90
_cell_angle_beta                        99.080(1)
_cell_angle_gamma                       90
_cell_volume                           5606.7(8)
_cell_formula_units_Z                   4

_cell_measurement_temperature    200(1)
_cell_measurement_reflns_used      6207
_cell_measurement_theta_min        2.54
_cell_measurement_theta_max       21.02
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   6207 reflections after integration using the SAINT software
   package (Bruker, 2001).

 Reduced cell calculations did not indicate any higher metric lattice symmetry
   and examination of the final atomic coordinates of the structure did not
   yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description       'block'
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_exptl_crystal_size_max           0.48
_exptl_crystal_size_mid           0.22
_exptl_crystal_size_min           0.21
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.136
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2072
_exptl_absorpt_coefficient_mu     0.196
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, (Bruker, 2001))'
_exptl_absorpt_correction_T_min   0.8176
_exptl_absorpt_correction_T_max   0.9599

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# 7. EXPERIMENTAL DATA

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; ?
;
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_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
```

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;
_diffrn_measurement_method           'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2001)).
;
_diffrn_detector_area_resol_mean     66.06

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_diffrn_standards_interval_count     ?
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loop_
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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              39473
_diffrn_reflns_av_R_equivalents    0.0517
_diffrn_reflns_av_sigmaI/netI      0.0701
_diffrn_reflns_limit_h_min         -14
_diffrn_reflns_limit_h_max         14
_diffrn_reflns_limit_k_min         -26
_diffrn_reflns_limit_k_max         26
_diffrn_reflns_limit_l_min         -25
_diffrn_reflns_limit_l_max         25
_diffrn_reflns_theta_min           2.31
_diffrn_reflns_theta_max           25.03
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_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.999

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

# number of unique reflections
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_reflns_number_gt                  6372
_reflns_threshold_expression       I>2\s(I)


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_computing_data_reduction           'SAINT-Pus'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 2003)
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_computing_publication_material      'PLATON (Spek, 2003)'

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# 8. REFINEMENT DATA


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

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0628P)^2^+3.5283P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
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_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?

_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          9881
_refine_ls_number_parameters      627
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.1015
_refine_ls_R_factor_gt            0.0588
_refine_ls_wR_factor_ref          0.1699
_refine_ls_wR_factor_gt           0.1473
_refine_ls_goodness_of_fit_ref    1.022
_refine_ls_restrained_S_all       1.022
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000
 _refine_diff_density_max          0.302
_refine_diff_density_min         -0.292
_refine_diff_density_rms          0.043

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_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Ti1 Ti Uani 0.17496(4) 0.24274(3) 0.39936(2) 1.000 0.0454(2) . .
O1 O Uani 0.20983(17) 0.17255(10) 0.46714(10) 1.000 0.0572(8) . .
C11 C Uani 0.2285(3) 0.34716(16) 0.39325(15) 1.000 0.0586(11) . .
C12 C Uani 0.3048(3) 0.31435(15) 0.36176(14) 1.000 0.0550(11) . .
C13 C Uani 0.3723(3) 0.27561(17) 0.40587(15) 1.000 0.0614(13) . .
C14 C Uani 0.3363(3) 0.28530(18) 0.46482(15) 1.000 0.0641(13) . .
C15 C Uani 0.2449(3) 0.32796(17) 0.45642(15) 1.000 0.0606(11) . .
C16 C Uani 0.1570(3) 0.40012(16) 0.36595(19) 1.000 0.0768(16) . .
C17 C Uani 0.3280(3) 0.32963(17) 0.29714(15) 1.000 0.0668(14) . .
C18 C Uani 0.4741(3) 0.2383(2) 0.39430(18) 1.000 0.0808(16) . .
C19 C Uani 0.3951(3) 0.2612(2) 0.52681(18) 1.000 0.0953(19) . .
C110 C Uani 0.1885(4) 0.3550(2) 0.50812(19) 1.000 0.0879(17) . .
C111 C Uani 0.2936(3) 0.1232(2) 0.47020(18) 1.000 0.0869(17) . .
C112 C Uani 0.2864(4) 0.08945(17) 0.52779(18) 1.000 0.0785(16) . .
C113 C Uani 0.2174(3) 0.12762(18) 0.56569(16) 1.000 0.0709(14) . .
C114 C Uani 0.1438(3) 0.16513(19) 0.51874(16) 1.000 0.0713(14) . .
C115 C Uani 0.0093(2) 0.18631(15) 0.37635(14) 1.000 0.0500(11) . .
C116 C Uani -0.0294(2) 0.23532(15) 0.40786(15) 1.000 0.0525(11) . .
C117 C Uani -0.0134(2) 0.28759(15) 0.37416(15) 1.000 0.0529(11) . .
C118 C Uani 0.0348(2) 0.27156(14) 0.32131(14) 1.000 0.0471(10) . .
C119 C Uani 0.0531(2) 0.20745(14) 0.32168(14) 1.000 0.0460(10) . .
C120 C Uani 0.1474(3) 0.17985(14) 0.29911(14) 1.000 0.0507(11) . .
C121 C Uani 0.1800(3) 0.20059(14) 0.23717(14) 1.000 0.0505(10) . .
C122 C Uani 0.0963(3) 0.16949(15) 0.18450(16) 1.000 0.0647(12) . .
C123 C Uani 0.1076(4) 0.10093(17) 0.1900(2) 1.000 0.0815(16) . .
C124 C Uani 0.0809(4) 0.08043(17) 0.2537(2) 1.000 0.0867(16) . .
C125 C Uani 0.1651(3) 0.11195(16) 0.30621(18) 1.000 0.0687(14) . .
C126 C Uani 0.3031(3) 0.18170(16) 0.23074(16) 1.000 0.0625(12) . .
C127 C Uani 0.3161(4) 0.11388(18) 0.23657(19) 1.000 0.0775(17) . .
C128 C Uani 0.2322(4) 0.08307(18) 0.1847(2) 1.000 0.0939(18) . .
C129 C Uani 0.2901(3) 0.09466(18) 0.30102(19) 1.000 0.0816(16) . .
C21 C Uani 0.3134(2) 0.29727(13) 0.06284(13) 1.000 0.0420(9) . .
C22 C Uani 0.4173(2) 0.27094(14) 0.09073(14) 1.000 0.0476(10) . .
C23 C Uani 0.4452(3) 0.21102(16) 0.08167(16) 1.000 0.0583(11) . .
C24 C Uani 0.3697(3) 0.17371(16) 0.04397(17) 1.000 0.0646(14) . .
C25 C Uani 0.2663(3) 0.19797(16) 0.01540(17) 1.000 0.0640(12) . .
C26 C Uani 0.2395(3) 0.25776(14) 0.02465(16) 1.000 0.0542(11) . .
C27 C Uani 0.1777(2) 0.37266(12) 0.11962(13) 1.000 0.0392(9) . .
C28 C Uani 0.1014(2) 0.32596(13) 0.12810(13) 1.000 0.0420(9) . .
C29 C Uani 0.0128(2) 0.33317(14) 0.16322(13) 1.000 0.0468(10) . .
C210 C Uani -0.0026(2) 0.38743(14) 0.19136(14) 1.000 0.0487(10) . .
C211 C Uani 0.0720(3) 0.43417(14) 0.18508(15) 1.000 0.0533(11) . .
C212 C Uani 0.1600(3) 0.42649(14) 0.14978(14) 1.000 0.0493(11) . .
C213 C Uani 0.2150(2) 0.39299(12) 0.00245(13) 1.000 0.0408(9) . .
C214 C Uani 0.1088(2) 0.42342(13) -0.01009(14) 1.000 0.0455(10) . .
C215 C Uani 0.0621(3) 0.44290(14) -0.06931(15) 1.000 0.0515(11) . .
C216 C Uani 0.1192(3) 0.43297(15) -0.11942(15) 1.000 0.0567(11) . .
C217 C Uani 0.2247(3) 0.40331(15) -0.10913(14) 1.000 0.0544(11) . .
C218 C Uani 0.2703(2) 0.38445(14) -0.04943(14) 1.000 0.0471(10) . .
C219 C Uani 0.3850(2) 0.41034(12) 0.10107(13) 1.000 0.0407(9) . .
C220 C Uani 0.4277(2) 0.45863(13) 0.07056(14) 1.000 0.0467(10) . .
C221 C Uani 0.5193(3) 0.49468(15) 0.09847(16) 1.000 0.0558(11) . .
C222 C Uani 0.5720(3) 0.48287(15) 0.15849(16) 1.000 0.0572(11) . .
C223 C Uani 0.5324(3) 0.43552(15) 0.19112(15) 1.000 0.0565(11) . .
```

```
C224 C Uani 0.4409(2) 0.40056(14) 0.16300(14) 1.000 0.0490(10) . .
B2 B Uani 0.2745(3) 0.36800(15) 0.07188(15) 1.000 0.0399(10) . .
C51 C Uani 0.431(2) 0.4802(9) 0.4530(7) 1.000 0.336(10) . .
C52 C Uani 0.515(2) 0.4434(4) 0.4852(12) 1.000 0.333(14) . .
C53 C Uani 0.3996(18) 0.5165(18) 0.5022(15) 1.000 0.51(2) . .
O3 O Uani 0.7527(3) 0.2447(2) 0.1809(2) 1.000 0.1295(19) . .
C31 C Uani 0.7273(4) 0.2918(3) 0.2192(3) 1.000 0.110(2) . .
C32 C Uani 0.6564(5) 0.2678(3) 0.2637(3) 1.000 0.144(3) . .
C33 C Uani 0.6515(6) 0.2045(4) 0.2543(4) 1.000 0.169(4) . .
C34 C Uani 0.7403(5) 0.1916(3) 0.2139(3) 1.000 0.138(3) . .
O4 O Uani 0.8221(15) 0.4433(5) 0.3702(12) 1.000 0.385(12) . .
C41 C Uani 0.8958(12) 0.4731(10) 0.4137(4) 1.000 0.269(11) . .
C42 C Uani 0.7871(15) 0.4852(13) 0.3240(8) 1.000 0.392(16) . .
C43 C Uani 0.9270(9) 0.5303(6) 0.3801(9) 1.000 0.266(8) . .
C44 C Uani 0.886(2) 0.5154(6) 0.3205(10) 1.000 0.312(12) . .


H110' H Uiso 0.11202 0.37020 0.49069 1.000 0.1318 . .
H110" H Uiso 0.23581 0.38820 0.52771 1.000 0.1318 . .
H111' H Uiso 0.27503 0.09653 0.43342 1.000 0.1042 . .
H112' H Uiso 0.24803 0.05014 0.51788 1.000 0.0939 . .
H113' H Uiso 0.26840 0.15318 0.59554 1.000 0.0849 . .
H114' H Uiso 0.12814 0.20474 0.53661 1.000 0.0856 . .
H122' H Uiso 0.11382 0.18262 0.14347 1.000 0.0773 . .
H124' H Uiso 0.00058 0.09099 0.25745 1.000 0.1041 . .
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H128' H Uiso 0.24997 0.09540 0.14346 1.000 0.1125 . .
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H16 H Uiso 0.20718 0.43490 0.36310 1.000 0.1150 . .
H16' H Uiso 0.10021 0.41017 0.39281 1.000 0.1150 . .
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H17' H Uiso 0.36622 0.29553 0.28036 1.000 0.0999 . .
H17" H Uiso 0.37764 0.36524 0.29917 1.000 0.0999 . .
H18 H Uiso 0.54429 0.26261 0.40315 1.000 0.1215 . .
H18' H Uiso 0.46284 0.22529 0.35066 1.000 0.1215 . .
H18" H Uiso 0.48120 0.20291 0.42156 1.000 0.1215 . .
H19 H Uiso 0.44787 0.29178 0.54756 1.000 0.1430 . .
H19' H Uiso 0.43847 0.22478 0.51999 1.000 0.1430 . .
H19" H Uiso 0.33720 0.25151 0.55308 1.000 0.1430 . .
H110 H Uiso 0.18111 0.32399 0.53939 1.000 0.1318 . .
H111 H Uiso 0.37212 0.13938 0.47107 1.000 0.1042 . .
H112 H Uiso 0.36424 0.08204 0.55122 1.000 0.0939 . .
H113 H Uiso 0.16989 0.10216 0.58908 1.000 0.0849 . .
H114 H Uiso 0.06967 0.14474 0.50416 1.000 0.0856 . .
H115 H Uiso 0.00715 0.14539 0.38896 1.000 0.0599 . .
H116 H Uiso -0.06098 0.23346 0.44545 1.000 0.0631 . .
H117 H Uiso -0.03203 0.32737 0.38523 1.000 0.0632 . .
H118 H Uiso 0.05252 0.29866 0.29033 1.000 0.0564 . .
H121 H Uiso 0.17211 0.24535 0.23330 1.000 0.0606 . .
H122 H Uiso 0.01633 0.18153 0.18729 1.000 0.0773 . .
H123 H Uiso 0.05313 0.08125 0.15593 1.000 0.0980 . .
H124 H Uiso 0.08941 0.03616 0.25757 1.000 0.1041 . .
H125 H Uiso 0.14728 0.09893 0.34771 1.000 0.0823 . .
H126 H Uiso 0.32064 0.19486 0.18972 1.000 0.0747 . .
H127 H Uiso 0.39669 0.10229 0.23268 1.000 0.0928 . .
H128 H Uiso 0.24084 0.03879 0.18830 1.000 0.1125 . .
H129 H Uiso 0.34379 0.11506 0.33420 1.000 0.0976 . .
H22 H Uiso 0.47103 0.29519 0.11702 1.000 0.0570 . .
H23 H Uiso 0.51688 0.19553 0.10157 1.000 0.0699 . .
H24 H Uiso 0.38820 0.13270 0.03789 1.000 0.0775 . .
```

```
H25 H Uiso 0.21319 0.17334 -0.01085 1.000 0.0769 . .
H26 H Uiso 0.16784 0.27285 0.00425 1.000 0.0649 . .
H28 H Uiso 0.11043 0.28800 0.10924 1.000 0.0504 . .
H29 H Uiso -0.03720 0.30041 0.16770 1.000 0.0561 . .
H210 H Uiso -0.06361 0.39264 0.21475 1.000 0.0582 . .
H211 H Uiso 0.06332 0.47169 0.20487 1.000 0.0640 . .
H212 H Uiso 0.21013 0.45938 0.14611 1.000 0.0591 . .
H214 H Uiso 0.06756 0.43086 0.02336 1.000 0.0546 . .
H215 H Uiso -0.00972 0.46327 -0.07556 1.000 0.0617 . .
H216 H Uiso 0.08692 0.44613 -0.16004 1.000 0.0683 . .
H217 H Uiso 0.26536 0.39603 -0.14285 1.000 0.0652 . .
H218 H Uiso 0.34280 0.36471 -0.04343 1.000 0.0565 . .
H220 H Uiso 0.39316 0.46748 0.02903 1.000 0.0560 . .
H221 H Uiso 0.54515 0.52730 0.07596 1.000 0.0670 . .
H222 H Uiso 0.63482 0.50685 0.17736 1.000 0.0688 . .
H223 H Uiso 0.56776 0.42707 0.23260 1.000 0.0676 . .
H224 H Uiso 0.41453 0.36867 0.18629 1.000 0.0588 . .
H51 H Uiso 0.36494 0.45637 0.43214 1.000 0.4004 . .
H51' H Uiso 0.46198 0.50505 0.42166 1.000 0.4004 . .
H52 H Uiso 0.49178 0.42686 0.52361 1.000 0.3977 . .
H52' H Uiso 0.53581 0.40995 0.45888 1.000 0.3977 . .
H53 H Uiso 0.32530 0.53707 0.48843 1.000 0.6134 . .
H53' H Uiso 0.39309 0.49168 0.53927 1.000 0.6134 . .
H31 H Uiso 0.68490 0.32402 0.19367 1.000 0.1320 . .
H31' H Uiso 0.79925 0.30919 0.24199 1.000 0.1320 . .
H32 H Uiso 0.69171 0.27737 0.30706 1.000 0.1730 . .
H32' H Uiso 0.57822 0.28545 0.25582 1.000 0.1730 . .
H33 H Uiso 0.57423 0.19207 0.23334 1.000 0.2032 . .
H33' H Uiso 0.66938 0.18281 0.29449 1.000 0.2032 . .
H34 H Uiso 0.81419 0.18023 0.23966 1.000 0.1657 . .
H34' H Uiso 0.71496 0.15809 0.18480 1.000 0.1657 . .
H41 H Uiso 0.96514 0.44848 0.42799 1.000 0.3205 . .
H41' H Uiso 0.85865 0.48342 0.45016 1.000 0.3205 . .
H42 H Uiso 0.75694 0.46534 0.28393 1.000 0.4688 . .
H42' H Uiso 0.72743 0.51237 0.33582 1.000 0.4688 . .
H43 H Uiso 0.88823 0.56634 0.39376 1.000 0.3192 . .
H43' H Uiso 1.01108 0.53708 0.38635 1.000 0.3192 . .
H44 H Uiso 0.86998 0.55196 0.29434 1.000 0.3729 . .
H44' H Uiso 0.94068 0.48957 0.30263 1.000 0.3729 . .

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
Ti1 0.0372(3) 0.0602(4) 0.0400(3) 0.0146(3) 0.0103(2) 0.0015(2)
O1 0.0495(12) 0.0762(15) 0.0504(13) 0.0256(11) 0.0222(10) 0.0152(11)
C11 0.0522(18) 0.070(2) 0.054(2) 0.0076(17) 0.0092(16) -0.0120(17)
C12 0.0489(17) 0.073(2) 0.0426(18) 0.0137(16) 0.0054(14) -0.0167(16)
C13 0.0378(16) 0.095(3) 0.052(2) 0.0194(19) 0.0090(14) -0.0090(17)
C14 0.0470(18) 0.100(3) 0.0438(19) 0.0176(19) 0.0028(15) -0.0173(19)
C15 0.0556(19) 0.081(2) 0.047(2) -0.0004(17) 0.0133(16) -0.0187(18)
C16 0.089(3) 0.058(2) 0.082(3) 0.007(2) 0.009(2) -0.008(2)
C17 0.073(2) 0.081(3) 0.048(2) 0.0167(18) 0.0145(17) -0.0220(19)
C18 0.0417(18) 0.133(4) 0.069(2) 0.031(2) 0.0129(17) 0.006(2)
C19 0.066(2) 0.165(5) 0.051(2) 0.032(3) -0.0029(18) -0.023(3)
C110 0.093(3) 0.107(3) 0.069(3) -0.019(2) 0.029(2) -0.028(3)
C111 0.089(3) 0.109(3) 0.068(3) 0.036(2) 0.029(2) 0.054(2)
```

```
C112 0.101(3) 0.064(2) 0.071(3) 0.020(2) 0.015(2) 0.011(2)
C113 0.069(2) 0.093(3) 0.053(2) 0.024(2) 0.0167(18) -0.009(2)
C114 0.064(2) 0.101(3) 0.057(2) 0.029(2) 0.0350(18) 0.010(2)
C115 0.0419(16) 0.0543(19) 0.056(2) 0.0083(15) 0.0148(14) -0.0023(14)
C116 0.0367(15) 0.067(2) 0.056(2) 0.0005(17) 0.0144(14) 0.0014(14)
C117 0.0386(16) 0.061(2) 0.059(2) 0.0027(17) 0.0072(14) 0.0066(14)
C118 0.0429(16) 0.0520(19) 0.0443(18) 0.0065(14) 0.0009(14) 0.0031(14)
C119 0.0412(15) 0.0523(19) 0.0445(17) 0.0074(14) 0.0067(13) -0.0002(14)
C120 0.0547(18) 0.0508(19) 0.0500(19) 0.0133(15) 0.0187(15) 0.0065(14)
C121 0.0602(18) 0.0494(18) 0.0442(18) 0.0091(14) 0.0153(15) 0.0025(15)
C122 0.084(2) 0.060(2) 0.051(2) 0.0008(17) 0.0136(18) -0.0017(18)
C123 0.110(3) 0.060(2) 0.081(3) -0.009(2) 0.035(2) -0.014(2)
C124 0.119(3) 0.047(2) 0.107(3) 0.001(2) 0.058(3) -0.008(2)
C125 0.087(3) 0.058(2) 0.071(2) 0.0238(19) 0.043(2) 0.0162(19)
C126 0.068(2) 0.071(2) 0.055(2) 0.0131(17) 0.0301(17) 0.0079(18)
C127 0.093(3) 0.075(3) 0.075(3) 0.017(2) 0.046(2) 0.027(2)
C128 0.146(4) 0.054(2) 0.098(3) 0.004(2) 0.070(3) 0.013(3)
C129 0.103(3) 0.069(2) 0.085(3) 0.032(2) 0.053(2) 0.037(2)
C21 0.0366(14) 0.0483(17) 0.0442(17) 0.0058(14) 0.0157(12) 0.0021(13)
C22 0.0422(16) 0.057(2) 0.0460(18) 0.0055(14) 0.0144(13) 0.0047(14)
C23 0.0567(19) 0.065(2) 0.057(2) 0.0135(18) 0.0205(16) 0.0188(18)
C24 0.074(2) 0.049(2) 0.078(3) 0.0064(18) 0.034(2) 0.0122(18)
C25 0.065(2) 0.054(2) 0.075(2) -0.0125(18) 0.0170(19) -0.0071(17)
C26 0.0462(17) 0.0493(19) 0.067(2) -0.0038(16) 0.0086(16) 0.0026(14)
C27 0.0369(14) 0.0421(16) 0.0386(16) 0.0078(13) 0.0057(12) 0.0024(12)
C28 0.0395(15) 0.0449(17) 0.0417(17) 0.0059(13) 0.0070(12) 0.0004(13)
C29 0.0378(15) 0.057(2) 0.0460(18) 0.0109(15) 0.0083(13) -0.0052(14)
C210 0.0421(16) 0.063(2) 0.0440(18) 0.0086(16) 0.0163(13) 0.0073(15)
C211 0.0585(19) 0.0489(19) 0.057(2) -0.0006(15) 0.0228(16) 0.0065(15)
C212 0.0493(17) 0.0453(18) 0.058(2) 0.0025(15) 0.0231(15) -0.0033(14)
C213 0.0390(15) 0.0390(16) 0.0454(17) 0.0005(13) 0.0101(13) -0.0030(12)
C214 0.0410(15) 0.0473(18) 0.0494(19) 0.0026(14) 0.0109(13) 0.0006(13)
C215 0.0465(16) 0.0530(19) 0.053(2) 0.0061(15) 0.0019(15) 0.0039(14)
C216 0.060(2) 0.062(2) 0.0447(19) 0.0071(16) -0.0023(16) -0.0033(17)
C217 0.0557(19) 0.066(2) 0.0433(19) -0.0014(16) 0.0137(15) -0.0094(16)
C218 0.0413(15) 0.0562(19) 0.0451(18) 0.0010(15) 0.0109(13) 0.0021(14)
C219 0.0399(14) 0.0441(17) 0.0411(17) 0.0003(13) 0.0156(12) 0.0013(13)
C220 0.0494(16) 0.0485(18) 0.0444(17) 0.0018(14) 0.0142(14) -0.0037(14)
C221 0.0583(19) 0.054(2) 0.059(2) -0.0010(16) 0.0216(16) -0.0135(16)
C222 0.0490(18) 0.064(2) 0.060(2) -0.0159(17) 0.0134(16) -0.0118(16)
C223 0.0539(18) 0.072(2) 0.0438(19) -0.0064(17) 0.0085(15) -0.0026(17)
C224 0.0498(17) 0.0557(19) 0.0431(18) 0.0010(14) 0.0123(14) -0.0036(14)
B2 0.0371(16) 0.0440(19) 0.0407(19) 0.0028(15) 0.0131(14) 0.0001(14)
C51 0.40(2) 0.253(15) 0.268(14) 0.055(12) -0.211(15) -0.177(16)
C52 0.40(3) 0.088(7) 0.51(3) 0.000(10) 0.07(2) 0.013(10)
C53 0.204(17) 0.72(5) 0.64(4) -0.19(4) 0.15(2) 0.10(2)
O3 0.112(3) 0.146(4) 0.145(3) 0.001(3) 0.065(3) -0.012(2)
C31 0.083(3) 0.135(5) 0.122(4) 0.022(4) 0.048(3) 0.002(3)
C32 0.116(4) 0.189(7) 0.145(5) 0.042(5) 0.074(4) -0.010(4)
C33 0.140(5) 0.162(7) 0.222(8) 0.107(6) 0.078(5) 0.013(5)
C34 0.109(4) 0.121(5) 0.182(7) 0.035(5) 0.015(4) 0.016(4)
O4 0.40(2) 0.189(8) 0.58(3) 0.079(13) 0.118(19) 0.002(10)
C41 0.217(12) 0.49(3) 0.106(6) 0.144(11) 0.046(7) 0.148(14)
C42 0.296(18) 0.58(4) 0.241(17) -0.04(2) -0.138(15) -0.13(3)
C43 0.226(10) 0.287(16) 0.307(16) -0.221(15) 0.110(11) -0.097(10)
C44 0.53(3) 0.163(10) 0.316(19) 0.050(11) 0.29(2) 0.067(13)

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

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

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Ti1     O1         2.138(2)                    .      .                   yes
 Ti1     C11        2.411(4)                    .      .                   yes
 Ti1     C12        2.434(3)                    .      .                   yes
 Ti1     C13        2.418(4)                    .      .                   yes
 Ti1     C14        2.382(4)                    .      .                   yes
 Ti1     C15        2.339(4)                    .      .                   yes
 Ti1     C115       2.306(3)                    .      .                   yes
 Ti1     C116       2.448(2)                    .      .                   yes
 Ti1     C117       2.414(3)                    .      .                   yes
 Ti1     C118       2.264(3)                    .      .                   yes
 Ti1     C119       2.181(3)                    .      .                   yes
 O1      C111       1.468(5)                    .      .                   yes
 O1      C114       1.471(4)                    .      .                   yes
 O3      C34        1.399(8)                    .      .                   yes
 O3      C31        1.398(8)                    .      .                   yes
 O4      C42         1.38(3)                    .      .                   yes
 O4      C41         1.35(3)                    .      .                   yes
 C11     C16        1.512(5)                    .      .                   no
 C11     C12        1.414(5)                    .      .                   no
 C11     C15        1.421(5)                    .      .                   no
 C12     C13        1.431(5)                    .      .                   no
 C12     C17        1.511(5)                    .      .                   no
 C13     C14        1.428(5)                    .      .                   no
 C13     C18        1.510(5)                    .      .                   no
 C14     C15        1.423(5)                    .      .                   no
 C14     C19        1.512(5)                    .      .                   no
 C15     C110       1.516(6)                    .      .                   no
 C111    C112       1.472(6)                    .      .                   no
 C112    C113       1.506(6)                    .      .                   no
 C113    C114       1.485(5)                    .      .                   no
 C115    C116       1.399(4)                    .      .                   no
 C115    C119       1.446(4)                    .      .                   no
 C16     H16'         0.9801                    .      .                   no
 C116    C117       1.400(5)                    .      .                   no
 C16     H16"         0.9801                    .      .                   no
 C16     H16          0.9800                    .      .                   no
 C17     H17          0.9803                    .      .                   no
 C117    C118       1.405(4)                    .      .                   no
 C17     H17"         0.9798                    .      .                   no
 C17     H17'         0.9798                    .      .                   no
 C118    C119       1.439(4)                    .      .                   no
 C18     H18"         0.9793                    .      .                   no
 C18     H18'         0.9799                    .      .                   no
 C18     H18          0.9803                    .      .                   no
 C19     H19"         0.9796                    .      .                   no
```

C19	H19	0.9806	.	.	no
C19	H19'	0.9798	.	.	no
C119	C120	1.422(4)	.	.	no
C120	C125	1.526(5)	.	.	no
C120	C121	1.528(4)	.	.	no
C121	C122	1.550(5)	.	.	no
C121	C126	1.536(5)	.	.	no
C122	C123	1.530(5)	.	.	no
C123	C124	1.536(6)	.	.	no
C123	C128	1.542(7)	.	.	no
C124	C125	1.555(6)	.	.	no
C125	C129	1.542(5)	.	.	no
C126	C127	1.516(5)	.	.	no
C127	C129	1.540(6)	.	.	no
C127	C128	1.537(6)	.	.	no
C110	H110'	0.9801	.	.	no
C110	H110	0.9805	.	.	no
C110	H110"	0.9796	.	.	no
C111	H111	0.9893	.	.	no
C111	H111'	0.9907	.	.	no
C112	H112	0.9895	.	.	no
C112	H112'	0.9904	.	.	no
C113	H113	0.9901	.	.	no
C113	H113'	0.9900	.	.	no
C114	H114	0.9899	.	.	no
C114	H114'	0.9900	.	.	no
C115	H115	0.9501	.	.	no
C116	H116	0.9502	.	.	no
C117	H117	0.9498	.	.	no
C118	H118	0.9501	.	.	no
C121	H121	1.0000	.	.	no
C21	B2	1.656(4)	.	.	yes
C21	C26	1.410(4)	.	.	no
C21	C22	1.404(4)	.	.	no
C122	H122'	0.9900	.	.	no
C22	C23	1.391(5)	.	.	no
C122	H122	0.9899	.	.	no
C23	C24	1.385(5)	.	.	no
C123	H123	1.0001	.	.	no
C124	H124	0.9898	.	.	no
C124	H124'	0.9902	.	.	no
C24	C25	1.385(5)	.	.	no
C25	C26	1.386(5)	.	.	no
C125	H125	1.0001	.	.	no
C126	H126	0.9901	.	.	no
C126	H126'	0.9900	.	.	no
C27	B2	1.661(4)	.	.	yes
C127	H127	0.9996	.	.	no
C27	C212	1.394(4)	.	.	no
C27	C28	1.403(4)	.	.	no
C128	H128'	0.9903	.	.	no
C128	H128	0.9898	.	.	no
C28	C29	1.396(4)	.	.	no
C129	H129	0.9902	.	.	no
C129	H129'	0.9900	.	.	no
C29	C210	1.375(4)	.	.	no
C22	H22	0.9498	.	.	no
C23	H23	0.9499	.	.	no
C24	H24	0.9499	.	.	no
C25	H25	0.9501	.	.	no
C26	H26	0.9501	.	.	no

C28	H28	0.9501	.	.	no
C29	H29	0.9502	.	.	no
C210	C211	1.380(4)	.	.	no
C211	C212	1.394(5)	.	.	no
C213	C214	1.410(4)	.	.	no
C213	C218	1.401(4)	.	.	no
C213	B2	1.655(4)	.	.	yes
C214	C215	1.386(4)	.	.	no
C215	C216	1.385(5)	.	.	no
C216	C217	1.393(5)	.	.	no
C217	C218	1.388(4)	.	.	no
C219	C224	1.418(4)	.	.	no
C219	B2	1.649(4)	.	.	yes
C219	C220	1.395(4)	.	.	no
C220	C221	1.402(4)	.	.	no
C221	C222	1.378(5)	.	.	no
C222	C223	1.389(5)	.	.	no
C223	C224	1.389(4)	.	.	no
C51	C52	1.38(3)	.	.	no
C51	C53	1.43(4)	.	.	no
C52	C53	1.34(4)	.	3_666	no
C210	H210	0.9503	.	.	no
C211	H211	0.9500	.	.	no
C212	H212	0.9500	.	.	no
C214	H214	0.9501	.	.	no
C215	H215	0.9496	.	.	no
C216	H216	0.9501	.	.	no
C217	H217	0.9501	.	.	no
C218	H218	0.9501	.	.	no
C220	H220	0.9499	.	.	no
C221	H221	0.9502	.	.	no
C222	H222	0.9502	.	.	no
C223	H223	0.9499	.	.	no
C224	H224	0.9502	.	.	no
C51	H51'	0.9896	.	.	no
C51	H51	0.9894	.	.	no
C52	H52	0.9889	.	.	no
C52	H52'	0.9911	.	.	no
C53	H53	0.9904	.	.	no
C53	H53'	0.9886	.	.	no
C31	C32	1.473(9)	.	.	no
C32	C33	1.419(11)	.	.	no
C33	C34	1.495(10)	.	.	no
C31	H31	0.9904	.	.	no
C31	H31'	0.9897	.	.	no
C32	H32'	0.9902	.	.	no
C32	H32	0.9909	.	.	no
C33	H33	0.9903	.	.	no
C33	H33'	0.9902	.	.	no
C34	H34'	0.9911	.	.	no
C34	H34	0.9901	.	.	no
C41	C43	1.54(2)	.	.	no
C42	C44	1.36(3)	.	.	no
C43	C44	1.35(3)	.	.	no
C41	H41	0.9908	.	.	no
C41	H41'	0.9903	.	.	no
C42	H42	0.9903	.	.	no
C42	H42'	0.9901	.	.	no
C43	H43	0.9895	.	.	no
C43	H43'	0.9894	.	.	no
C44	H44	0.9915	.	.	no

```
 C44     H44'         0.9863                    .       .                 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
 O1      Ti1     C11      135.62(10)              .       .       .          yes
 O1      Ti1     C12      130.11(10)              .       .       .          yes
 O1      Ti1     C13       95.81(10)              .       .       .          yes
 O1      Ti1     C14       80.17(11)              .       .       .          yes
 O1      Ti1     C15      102.17(10)              .       .       .          yes
 O1      Ti1     C115      79.49(10)              .       .       .          yes
 O1      Ti1     C116      89.04(10)              .       .       .          yes
 O1      Ti1     C117      121.75(9)              .       .       .          yes
 O1      Ti1     C118     139.44(10)              .       .       .          yes
 O1      Ti1     C119     107.62(10)              .       .       .          yes
 C11     Ti1     C12       33.94(11)              .       .       .          yes
 C11     Ti1     C13       57.05(12)              .       .       .          yes
 C11     Ti1     C14       57.37(12)              .       .       .          yes
 C11     Ti1     C15       34.77(11)              .       .       .          yes
 C11     Ti1     C115     136.88(12)              .       .       .          yes
 C11     Ti1     C116     109.73(12)              .       .       .          yes
 C11     Ti1     C117      80.22(11)              .       .       .          yes
 C11     Ti1     C118      81.56(11)              .       .       .          yes
 C11     Ti1     C119     116.64(12)              .       .       .          yes
 C12     Ti1     C13       34.31(11)              .       .       .          yes
 C12     Ti1     C14       57.13(11)              .       .       .          yes
 C12     Ti1     C15       57.49(11)              .       .       .          yes
 C12     Ti1     C115     146.79(11)              .       .       .          yes
 C12     Ti1     C116     138.27(11)              .       .       .          yes
 C12     Ti1     C117     104.95(11)              .       .       .          yes
 C12     Ti1     C118      89.23(11)              .       .       .          yes
 C12     Ti1     C119     110.26(11)              .       .       .          yes
 C13     Ti1     C14       34.59(11)              .       .       .          yes
 C13     Ti1     C15       58.02(12)              .       .       .          yes
 C13     Ti1     C115     161.59(12)              .       .       .          yes
 C13     Ti1     C116     164.33(12)              .       .       .          yes
 C13     Ti1     C117     136.80(12)              .       .       .          yes
 C13     Ti1     C118     122.60(11)              .       .       .          yes
 C13     Ti1     C119     131.48(11)              .       .       .          yes
 C14     Ti1     C15       35.09(13)              .       .       .          yes
 C14     Ti1     C115     155.90(11)              .       .       .          yes
 C14     Ti1     C116     133.06(11)              .       .       .          yes
 C14     Ti1     C117     126.14(12)              .       .       .          yes
 C14     Ti1     C118     138.93(12)              .       .       .          yes
 C14     Ti1     C119     165.94(11)              .       .       .          yes
 C15     Ti1     C115     140.29(12)              .       .       .          yes
 C15     Ti1     C116     106.41(12)              .       .       .          yes
 C15     Ti1     C117      91.20(12)              .       .       .          yes
 C15     Ti1     C118     108.83(12)              .       .       .          yes
 C15     Ti1     C119     146.54(12)              .       .       .          yes
 C115    Ti1     C116      34.07(11)              .       .       .          yes
 C115    Ti1     C117      57.25(11)              .       .       .          yes
 C115    Ti1     C118      59.95(11)              .       .       .          yes
 C115    Ti1     C119      37.47(10)              .       .       .          yes
 C116    Ti1     C117      33.47(11)              .       .       .          yes
```

C116	Ti1	C118	57.75(10)	.	.	.	yes
C116	Ti1	C119	59.98(10)	.	.	.	yes
C117	Ti1	C118	34.76(10)	.	.	.	yes
C117	Ti1	C119	60.25(11)	.	.	.	yes
C118	Ti1	C119	37.72(11)	.	.	.	yes
Ti1	O1	C111	129.0(2)	.	.	.	yes
Ti1	O1	C114	122.6(2)	.	.	.	yes
C111	O1	C114	108.3(3)	.	.	.	yes
C31	O3	C34	106.0(5)	.	.	.	yes
C41	O4	C42	105.3(15)	.	.	.	yes
Ti1	C11	C15	69.8(2)	.	.	.	yes
Ti1	C11	C12	73.9(2)	.	.	.	yes
C12	C11	C16	124.6(3)	.	.	.	no
Ti1	C11	C16	129.4(2)	.	.	.	yes
C12	C11	C15	108.2(3)	.	.	.	no
C15	C11	C16	126.5(3)	.	.	.	no
Ti1	C12	C13	72.2(2)	.	.	.	yes
Ti1	C12	C17	132.4(2)	.	.	.	yes
C11	C12	C17	123.8(3)	.	.	.	no
C13	C12	C17	126.5(3)	.	.	.	no
C11	C12	C13	108.3(3)	.	.	.	no
Ti1	C12	C11	72.1(2)	.	.	.	yes
Ti1	C13	C14	71.3(2)	.	.	.	yes
Ti1	C13	C18	127.3(3)	.	.	.	yes
C12	C13	C18	126.1(3)	.	.	.	no
C14	C13	C18	126.0(3)	.	.	.	no
Ti1	C13	C12	73.5(2)	.	.	.	yes
C12	C13	C14	107.3(3)	.	.	.	no
Ti1	C14	C19	127.0(3)	.	.	.	yes
Ti1	C14	C13	74.1(2)	.	.	.	yes
Ti1	C14	C15	70.8(2)	.	.	.	yes
C15	C14	C19	125.5(3)	.	.	.	no
C13	C14	C15	108.1(3)	.	.	.	no
C13	C14	C19	125.9(3)	.	.	.	no
Ti1	C15	C14	74.1(2)	.	.	.	yes
Ti1	C15	C110	123.6(3)	.	.	.	yes
C11	C15	C110	126.0(3)	.	.	.	no
C14	C15	C110	125.4(3)	.	.	.	no
C11	C15	C14	107.9(3)	.	.	.	no
Ti1	C15	C11	75.4(2)	.	.	.	yes
O1	C111	C112	106.8(3)	.	.	.	yes
C111	C112	C113	106.7(3)	.	.	.	no
C112	C113	C114	104.3(3)	.	.	.	no
O1	C114	C113	105.4(3)	.	.	.	yes
Ti1	C115	C119	66.58(15)	.	.	.	yes
Ti1	C115	C116	78.55(17)	.	.	.	yes
C116	C115	C119	109.6(3)	.	.	.	no
Ti1	C116	C117	71.93(14)	.	.	.	yes
Ti1	C116	C115	67.38(14)	.	.	.	yes
C11	C16	H16	109.46	.	.	.	no
C11	C16	H16'	109.48	.	.	.	no
C11	C16	H16"	109.48	.	.	.	no
H16	C16	H16'	109.47	.	.	.	no
H16	C16	H16"	109.47	.	.	.	no
C115	C116	C117	107.9(3)	.	.	.	no
H16'	C16	H16"	109.47	.	.	.	no
C12	C17	H17'	109.48	.	.	.	no
C12	C17	H17"	109.47	.	.	.	no
H17	C17	H17'	109.46	.	.	.	no
H17	C17	H17"	109.47	.	.	.	no
H17'	C17	H17"	109.51	.	.	.	no

Ti1	C117	C116	74.60(16)	.	.	.	yes
Ti1	C117	C118	66.77(15)	.	.	.	yes
C116	C117	C118	108.8(3)	.	.	.	no
C12	C17	H17	109.44	.	.	.	no
C13	C18	H18	109.42	.	.	.	no
C13	C18	H18"	109.47	.	.	.	no
Ti1	C118	C117	78.47(17)	.	.	.	yes
C13	C18	H18'	109.44	.	.	.	no
C117	C118	C119	109.0(3)	.	.	.	no
H18	C18	H18"	109.51	.	.	.	no
Ti1	C118	C119	68.01(16)	.	.	.	yes
H18	C18	H18'	109.46	.	.	.	no
H18'	C18	H18"	109.54	.	.	.	no
H19	C19	H19'	109.44	.	.	.	no
C118	C119	C120	123.3(3)	.	.	.	no
C14	C19	H19'	109.48	.	.	.	no
C14	C19	H19"	109.49	.	.	.	no
Ti1	C119	C115	75.95(17)	.	.	.	yes
H19'	C19	H19"	109.53	.	.	.	no
C115	C119	C118	104.7(2)	.	.	.	no
C115	C119	C120	122.9(3)	.	.	.	no
C14	C19	H19	109.43	.	.	.	no
H19	C19	H19"	109.45	.	.	.	no
Ti1	C119	C120	88.12(18)	.	.	.	yes
Ti1	C119	C118	74.27(17)	.	.	.	yes
C119	C120	C121	119.5(3)	.	.	.	no
C119	C120	C125	119.5(3)	.	.	.	no
C121	C120	C125	109.7(3)	.	.	.	no
C122	C121	C126	108.1(3)	.	.	.	no
C120	C121	C122	107.3(3)	.	.	.	no
C120	C121	C126	111.7(3)	.	.	.	no
C121	C122	C123	110.4(3)	.	.	.	no
C124	C123	C128	108.9(4)	.	.	.	no
C122	C123	C124	109.7(3)	.	.	.	no
C122	C123	C128	108.8(3)	.	.	.	no
C123	C124	C125	109.3(3)	.	.	.	no
C120	C125	C129	110.8(3)	.	.	.	no
C120	C125	C124	108.0(3)	.	.	.	no
C124	C125	C129	109.9(3)	.	.	.	no
C121	C126	C127	110.3(3)	.	.	.	no
C126	C127	C128	109.6(3)	.	.	.	no
C128	C127	C129	110.3(3)	.	.	.	no
C126	C127	C129	108.6(3)	.	.	.	no
C123	C128	C127	109.9(3)	.	.	.	no
C125	C129	C127	109.1(3)	.	.	.	no
C15	C110	H110	109.43	.	.	.	no
C15	C110	H110'	109.47	.	.	.	no
C15	C110	H110"	109.51	.	.	.	no
H110"	C110	H110	109.48	.	.	.	no
H110'	C110	H110"	109.51	.	.	.	no
H110'	C110	H110	109.43	.	.	.	no
C112	C111	H111'	110.28	.	.	.	no
C112	C111	H111	110.33	.	.	.	no
O1	C111	H111	110.44	.	.	.	no
H111'	C111	H111	108.60	.	.	.	no
O1	C111	H111'	110.36	.	.	.	no
C111	C112	H112'	110.42	.	.	.	no
C111	C112	H112	110.42	.	.	.	no
C113	C112	H112	110.38	.	.	.	no
H112'	C112	H112	108.62	.	.	.	no
C113	C112	H112'	110.33	.	.	.	no

C112	C113	H113	110.92	.	.	.	no
C114	C113	H113'	110.90	.	.	.	no
H113'	C113	H113	108.92	.	.	.	no
C114	C113	H113	110.89	.	.	.	no
C112	C113	H113'	110.90	.	.	.	no
O1	C114	H114'	110.68	.	.	.	no
C113	C114	H114	110.68	.	.	.	no
H114'	C114	H114	108.78	.	.	.	no
O1	C114	H114	110.66	.	.	.	no
C113	C114	H114'	110.67	.	.	.	no
C116	C115	H115	125.20	.	.	.	no
Ti1	C115	H115	121.12	.	.	.	no
C119	C115	H115	125.19	.	.	.	no
C115	C116	H116	126.06	.	.	.	no
C117	C116	H116	126.06	.	.	.	no
Ti1	C116	H116	126.19	.	.	.	no
C116	C117	H117	125.60	.	.	.	no
Ti1	C117	H117	124.51	.	.	.	no
C118	C117	H117	125.57	.	.	.	no
C117	C118	H118	125.53	.	.	.	no
Ti1	C118	H118	119.59	.	.	.	no
C119	C118	H118	125.49	.	.	.	no
C122	C121	H121	109.91	.	.	.	no
C126	C121	H121	109.87	.	.	.	no
C22	C21	B2	125.6(3)	.	.	.	yes
C26	C21	B2	120.2(2)	.	.	.	yes
C120	C121	H121	109.91	.	.	.	no
C22	C21	C26	114.2(3)	.	.	.	no
C121	C122	H122	109.57	.	.	.	no
C123	C122	H122'	109.57	.	.	.	no
C123	C122	H122	109.60	.	.	.	no
H122'	C122	H122	108.13	.	.	.	no
C121	C122	H122'	109.58	.	.	.	no
C21	C22	C23	123.1(3)	.	.	.	no
C22	C23	C24	120.8(3)	.	.	.	no
C122	C123	H123	109.80	.	.	.	no
C128	C123	H123	109.83	.	.	.	no
C124	C123	H123	109.82	.	.	.	no
C125	C124	H124'	109.88	.	.	.	no
C123	C124	H124	109.77	.	.	.	no
C125	C124	H124	109.88	.	.	.	no
H124'	C124	H124	108.25	.	.	.	no
C23	C24	C25	118.0(3)	.	.	.	no
C123	C124	H124'	109.76	.	.	.	no
C24	C25	C26	120.8(3)	.	.	.	no
C124	C125	H125	109.35	.	.	.	no
C129	C125	H125	109.42	.	.	.	no
C120	C125	H125	109.38	.	.	.	no
C121	C126	H126	109.58	.	.	.	no
C21	C26	C25	123.2(3)	.	.	.	no
C127	C126	H126	109.60	.	.	.	no
C127	C126	H126'	109.58	.	.	.	no
H126'	C126	H126	108.12	.	.	.	no
C121	C126	H126'	109.59	.	.	.	no
C129	C127	H127	109.46	.	.	.	no
C212	C27	B2	121.0(2)	.	.	.	yes
C126	C127	H127	109.45	.	.	.	no
C28	C27	C212	115.2(3)	.	.	.	no
C128	C127	H127	109.42	.	.	.	no
C28	C27	B2	123.6(2)	.	.	.	yes
C123	C128	H128	109.67	.	.	.	no

C123	C128	H128'	109.64	.	.	.	no
C127	C128	H128	109.73	.	.	.	no
C27	C28	C29	122.5(3)	.	.	.	no
C127	C128	H128'	109.71	.	.	.	no
H128'	C128	H128	108.19	.	.	.	no
C127	C129	H129	109.85	.	.	.	no
H129'	C129	H129	108.26	.	.	.	no
C127	C129	H129'	109.88	.	.	.	no
C28	C29	C210	120.4(3)	.	.	.	no
C125	C129	H129'	109.90	.	.	.	no
C125	C129	H129	109.88	.	.	.	no
C23	C22	H22	118.48	.	.	.	no
C21	C22	H22	118.43	.	.	.	no
C24	C23	H23	119.62	.	.	.	no
C22	C23	H23	119.62	.	.	.	no
C23	C24	H24	121.02	.	.	.	no
C25	C24	H24	120.98	.	.	.	no
C26	C25	H25	119.64	.	.	.	no
C24	C25	H25	119.61	.	.	.	no
C21	C26	H26	118.41	.	.	.	no
C25	C26	H26	118.40	.	.	.	no
C27	C28	H28	118.74	.	.	.	no
C29	C28	H28	118.79	.	.	.	no
C210	C29	H29	119.81	.	.	.	no
C28	C29	H29	119.81	.	.	.	no
C29	C210	C211	118.9(3)	.	.	.	no
C210	C211	C212	120.2(3)	.	.	.	no
C27	C212	C211	122.9(3)	.	.	.	no
C214	C213	C218	114.9(3)	.	.	.	no
C214	C213	B2	124.9(2)	.	.	.	yes
C218	C213	B2	120.3(2)	.	.	.	yes
C213	C214	C215	122.6(3)	.	.	.	no
C214	C215	C216	120.6(3)	.	.	.	no
C215	C216	C217	118.7(3)	.	.	.	no
C216	C217	C218	119.8(3)	.	.	.	no
C213	C218	C217	123.4(3)	.	.	.	no
C220	C219	B2	125.2(2)	.	.	.	yes
C220	C219	C224	114.9(2)	.	.	.	no
C224	C219	B2	119.9(2)	.	.	.	yes
C219	C220	C221	122.9(3)	.	.	.	no
C220	C221	C222	120.1(3)	.	.	.	no
C221	C222	C223	119.3(3)	.	.	.	no
C222	C223	C224	119.9(3)	.	.	.	no
C219	C224	C223	122.9(3)	.	.	.	no
C52	C51	C53	101.7(18)	.	.	.	no
C51	C52	C53	99.5(18)	.	.	3_666	no
C51	C53	C52	105(2)	.	.	3_666	no
C29	C210	H210	120.54	.	.	.	no
C211	C210	H210	120.55	.	.	.	no
C212	C211	H211	119.92	.	.	.	no
C210	C211	H211	119.90	.	.	.	no
C211	C212	H212	118.56	.	.	.	no
C27	C212	H212	118.56	.	.	.	no
C215	C214	H214	118.68	.	.	.	no
C213	C214	H214	118.71	.	.	.	no
C214	C215	H215	119.68	.	.	.	no
C216	C215	H215	119.70	.	.	.	no
C215	C216	H216	120.58	.	.	.	no
C217	C216	H216	120.69	.	.	.	no
C216	C217	H217	120.13	.	.	.	no
C218	C217	H217	120.11	.	.	.	no

C217	C218	H218	118.30	.	.	.	no
C213	C218	H218	118.28	.	.	.	no
C219	C220	H220	118.54	.	.	.	no
C221	C220	H220	118.54	.	.	.	no
C220	C221	H221	119.96	.	.	.	no
C222	C221	H221	119.93	.	.	.	no
C221	C222	H222	120.36	.	.	.	no
C223	C222	H222	120.32	.	.	.	no
C222	C223	H223	120.10	.	.	.	no
C224	C223	H223	120.04	.	.	.	no
C223	C224	H224	118.55	.	.	.	no
C219	C224	H224	118.52	.	.	.	no
C53	C51	H51	111.43	.	.	.	no
H51	C51	H51'	109.35	.	.	.	no
C52	C51	H51	111.32	.	.	.	no
C52	C51	H51'	111.40	.	.	.	no
C53	C51	H51'	111.50	.	.	.	no
C53	C52	H52	111.82	3_666	.	.	no
C51	C52	H52'	111.86	.	.	.	no
H52	C52	H52'	109.59	.	.	.	no
C53	C52	H52'	111.76	3_666	.	.	no
C51	C52	H52	112.01	.	.	.	no
C52	C53	H53	110.78	3_666	.	.	no
C52	C53	H53'	110.87	3_666	.	.	no
C51	C53	H53'	110.90	.	.	.	no
H53	C53	H53'	108.94	.	.	.	no
C51	C53	H53	110.70	.	.	.	no
O3	C31	C32	108.5(5)	.	.	.	yes
C31	C32	C33	106.1(6)	.	.	.	no
C32	C33	C34	104.9(6)	.	.	.	no
O3	C34	C33	106.2(6)	.	.	.	yes
O3	C31	H31'	110.05	.	.	.	no
C32	C31	H31'	109.98	.	.	.	no
H31	C31	H31'	108.35	.	.	.	no
C32	C31	H31	109.92	.	.	.	no
O3	C31	H31	110.06	.	.	.	no
C31	C32	H32'	110.56	.	.	.	no
H32	C32	H32'	108.59	.	.	.	no
C33	C32	H32'	110.55	.	.	.	no
C31	C32	H32	110.50	.	.	.	no
C33	C32	H32	110.51	.	.	.	no
C32	C33	H33	110.82	.	.	.	no
C32	C33	H33'	110.86	.	.	.	no
C34	C33	H33	110.71	.	.	.	no
C34	C33	H33'	110.70	.	.	.	no
H33	C33	H33'	108.79	.	.	.	no
O3	C34	H34'	110.51	.	.	.	no
C33	C34	H34'	110.49	.	.	.	no
H34	C34	H34'	108.58	.	.	.	no
C33	C34	H34	110.53	.	.	.	no
O3	C34	H34	110.54	.	.	.	no
O4	C41	C43	104.3(12)	.	.	.	yes
O4	C42	C44	102.3(16)	.	.	.	yes
C41	C43	C44	100.2(12)	.	.	.	no
C42	C44	C43	104.3(17)	.	.	.	no
C43	C41	H41	110.93	.	.	.	no
O4	C41	H41'	110.90	.	.	.	no
O4	C41	H41	110.85	.	.	.	no
C43	C41	H41'	110.96	.	.	.	no
H41	C41	H41'	108.85	.	.	.	no
O4	C42	H42	111.31	.	.	.	no

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 C44     C42     H42          111.26              .       .       .          no
 C44     C42     H42'         111.37              .       .       .          no
 H42     C42     H42'         109.17              .       .       .          no
 O4      C42     H42'         111.33              .       .       .          no
 C41     C43     H43'         111.67              .       .       .          no
 C44     C43     H43          111.94              .       .       .          no
 C41     C43     H43          111.65              .       .       .          no
 H43     C43     H43'         109.57              .       .       .          no
 C44     C43     H43'         111.57              .       .       .          no
 C42     C44     H44'         110.77              .       .       .          no
 C43     C44     H44          110.87              .       .       .          no
 H44     C44     H44'         109.08              .       .       .          no
 C43     C44     H44'         111.29              .       .       .          no
 C42     C44     H44          110.44              .       .       .          no
 C213    B2      C219       110.8(2)              .       .       .          yes
 C21     B2      C27        111.3(2)              .       .       .          yes
 C21     B2      C213       107.2(2)              .       .       .          yes
 C21     B2      C219       111.7(2)              .       .       .          yes
 C27     B2      C213       108.3(2)              .       .       .          yes
 C27     B2      C219       107.6(2)              .       .       .          yes

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
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_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 C11     Ti1     O1      C111       -99.6(3)     .       .       .       .   no
 C11     Ti1     O1      C114        84.0(3)     .       .       .       .   no
 C12     Ti1     O1      C111       -53.2(3)     .       .       .       .   no
 C12     Ti1     O1      C114       130.4(2)     .       .       .       .   no
 C13     Ti1     O1      C111       -52.2(3)     .       .       .       .   no
 C13     Ti1     O1      C114       131.3(2)     .       .       .       .   no
 C14     Ti1     O1      C111       -83.2(3)     .       .       .       .   no
 C14     Ti1     O1      C114       100.4(2)     .       .       .       .   no
 C15     Ti1     O1      C111      -110.7(3)     .       .       .       .   no
 C15     Ti1     O1      C114        72.9(2)     .       .       .       .   no
 C115    Ti1     O1      C111       109.8(3)     .       .       .       .   no
 C115    Ti1     O1      C114       -66.7(2)     .       .       .       .   no
 C116    Ti1     O1      C111       142.7(3)     .       .       .       .   no
 C116    Ti1     O1      C114       -33.7(2)     .       .       .       .   no
 C117    Ti1     O1      C111       150.2(3)     .       .       .       .   no
 C117    Ti1     O1      C114       -26.3(3)     .       .       .       .   no
 C118    Ti1     O1      C111       109.9(3)     .       .       .       .   no
 C118    Ti1     O1      C114       -66.6(3)     .       .       .       .   no
 C119    Ti1     O1      C111        84.7(3)     .       .       .       .   no
 C119    Ti1     O1      C114       -91.7(2)     .       .       .       .   no
 O1      Ti1     C11     C12         97.5(2)     .       .       .       .   no
 O1      Ti1     C11     C15        -19.4(3)     .       .       .       .   no
 O1      Ti1     C11     C16       -140.6(3)     .       .       .       .   no
 C12     Ti1     C11     C15       -116.9(3)     .       .       .       .   no
 C12     Ti1     C11     C16        121.9(4)     .       .       .       .   no
 C13     Ti1     C11     C12       36.89(18)     .       .       .       .   no
 C13     Ti1     C11     C15        -80.0(2)     .       .       .       .   no
 C13     Ti1     C11     C16        158.8(3)     .       .       .       .   no
 C14     Ti1     C11     C12         78.3(2)     .       .       .       .   no
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C14	Ti1	C11	C15	-38.6(2)	.	.	.	no
C14	Ti1	C11	C16	-159.8(4)	.	.	.	no
C15	Ti1	C11	C12	116.9(3)	.	.	.	no
C15	Ti1	C11	C16	-121.2(4)	.	.	.	no
C115	Ti1	C11	C12	-127.3(2)	.	.	.	no
C115	Ti1	C11	C15	115.8(2)	.	.	.	no
C115	Ti1	C11	C16	-5.4(4)	.	.	.	no
C116	Ti1	C11	C12	-152.52(18)	.	.	.	no
C116	Ti1	C11	C15	90.6(2)	.	.	.	no
C116	Ti1	C11	C16	-30.7(3)	.	.	.	no
C117	Ti1	C11	C12	-136.5(2)	.	.	.	no
C117	Ti1	C11	C15	106.6(2)	.	.	.	no
C117	Ti1	C11	C16	-14.6(3)	.	.	.	no
C118	Ti1	C11	C12	-101.30(19)	.	.	.	no
C118	Ti1	C11	C15	141.8(2)	.	.	.	no
C118	Ti1	C11	C16	20.6(3)	.	.	.	no
C119	Ti1	C11	C12	-87.0(2)	.	.	.	no
C119	Ti1	C11	C15	156.05(19)	.	.	.	no
C119	Ti1	C11	C16	34.8(3)	.	.	.	no
O1	Ti1	C12	C11	-115.0(2)	.	.	.	no
O1	Ti1	C12	C13	1.7(2)	.	.	.	no
O1	Ti1	C12	C17	125.3(3)	.	.	.	no
C11	Ti1	C12	C13	116.7(3)	.	.	.	no
C11	Ti1	C12	C17	-119.8(4)	.	.	.	no
C13	Ti1	C12	C11	-116.7(3)	.	.	.	no
C13	Ti1	C12	C17	123.5(4)	.	.	.	no
C14	Ti1	C12	C11	-79.1(2)	.	.	.	no
C14	Ti1	C12	C13	37.6(2)	.	.	.	no
C14	Ti1	C12	C17	161.2(4)	.	.	.	no
C15	Ti1	C12	C11	-37.08(19)	.	.	.	no
C15	Ti1	C12	C13	79.6(2)	.	.	.	no
C15	Ti1	C12	C17	-156.9(4)	.	.	.	no
C115	Ti1	C12	C11	96.7(2)	.	.	.	no
C115	Ti1	C12	C13	-146.6(2)	.	.	.	no
C115	Ti1	C12	C17	-23.1(4)	.	.	.	no
C116	Ti1	C12	C11	40.7(3)	.	.	.	no
C116	Ti1	C12	C13	157.42(19)	.	.	.	no
C116	Ti1	C12	C17	-79.0(4)	.	.	.	no
C117	Ti1	C12	C11	44.6(2)	.	.	.	no
C117	Ti1	C12	C13	161.29(19)	.	.	.	no
C117	Ti1	C12	C17	-75.2(3)	.	.	.	no
C118	Ti1	C12	C11	75.95(19)	.	.	.	no
C118	Ti1	C12	C13	-167.4(2)	.	.	.	no
C118	Ti1	C12	C17	-43.8(3)	.	.	.	no
C119	Ti1	C12	C11	107.93(19)	.	.	.	no
C119	Ti1	C12	C13	-135.39(19)	.	.	.	no
C119	Ti1	C12	C17	-11.9(3)	.	.	.	no
O1	Ti1	C13	C12	-178.68(18)	.	.	.	no
O1	Ti1	C13	C14	-63.3(2)	.	.	.	no
O1	Ti1	C13	C18	58.2(3)	.	.	.	no
C11	Ti1	C13	C12	-36.47(18)	.	.	.	no
C11	Ti1	C13	C14	78.9(2)	.	.	.	no
C11	Ti1	C13	C18	-159.6(3)	.	.	.	no
C12	Ti1	C13	C14	115.4(3)	.	.	.	no
C12	Ti1	C13	C18	-123.1(4)	.	.	.	no
C14	Ti1	C13	C12	-115.4(3)	.	.	.	no
C14	Ti1	C13	C18	121.5(4)	.	.	.	no
C15	Ti1	C13	C12	-77.9(2)	.	.	.	no
C15	Ti1	C13	C14	37.5(2)	.	.	.	no
C15	Ti1	C13	C18	158.9(3)	.	.	.	no
C117	Ti1	C13	C12	-26.9(3)	.	.	.	no

C117	Ti1	C13	C14	88.5(2)	.	.	.	no
C117	Ti1	C13	C18	-150.0(3)	.	.	.	no
C118	Ti1	C13	C12	15.1(2)	.	.	.	no
C118	Ti1	C13	C14	130.5(2)	.	.	.	no
C118	Ti1	C13	C18	-108.1(3)	.	.	.	no
C119	Ti1	C13	C12	61.6(2)	.	.	.	no
C119	Ti1	C13	C14	177.0(2)	.	.	.	no
C119	Ti1	C13	C18	-61.5(3)	.	.	.	no
O1	Ti1	C14	C13	115.6(2)	.	.	.	no
O1	Ti1	C14	C15	-128.2(2)	.	.	.	no
O1	Ti1	C14	C19	-7.8(3)	.	.	.	no
C11	Ti1	C14	C13	-77.9(2)	.	.	.	no
C11	Ti1	C14	C15	38.25(19)	.	.	.	no
C11	Ti1	C14	C19	158.7(4)	.	.	.	no
C12	Ti1	C14	C13	-37.3(2)	.	.	.	no
C12	Ti1	C14	C15	78.9(2)	.	.	.	no
C12	Ti1	C14	C19	-160.7(4)	.	.	.	no
C13	Ti1	C14	C15	116.2(3)	.	.	.	no
C13	Ti1	C14	C19	-123.4(4)	.	.	.	no
C15	Ti1	C14	C13	-116.2(3)	.	.	.	no
C15	Ti1	C14	C19	120.5(4)	.	.	.	no
C115	Ti1	C14	C13	148.4(3)	.	.	.	no
C115	Ti1	C14	C15	-95.5(3)	.	.	.	no
C115	Ti1	C14	C19	25.0(5)	.	.	.	no
C116	Ti1	C14	C13	-165.1(2)	.	.	.	no
C116	Ti1	C14	C15	-48.9(3)	.	.	.	no
C116	Ti1	C14	C19	71.6(4)	.	.	.	no
C117	Ti1	C14	C13	-122.1(2)	.	.	.	no
C117	Ti1	C14	C15	-5.9(2)	.	.	.	no
C117	Ti1	C14	C19	114.6(3)	.	.	.	no
C118	Ti1	C14	C13	-77.3(3)	.	.	.	no
C118	Ti1	C14	C15	38.8(3)	.	.	.	no
C118	Ti1	C14	C19	159.3(3)	.	.	.	no
O1	Ti1	C15	C11	166.27(19)	.	.	.	no
O1	Ti1	C15	C14	52.4(2)	.	.	.	no
O1	Ti1	C15	C110	-69.9(3)	.	.	.	no
C11	Ti1	C15	C14	-113.9(3)	.	.	.	no
C11	Ti1	C15	C110	123.8(4)	.	.	.	no
C12	Ti1	C15	C11	36.2(2)	.	.	.	no
C12	Ti1	C15	C14	-77.7(2)	.	.	.	no
C12	Ti1	C15	C110	160.0(3)	.	.	.	no
C13	Ti1	C15	C11	77.0(2)	.	.	.	no
C13	Ti1	C15	C14	-36.92(19)	.	.	.	no
C13	Ti1	C15	C110	-159.2(3)	.	.	.	no
C14	Ti1	C15	C11	113.9(3)	.	.	.	no
C14	Ti1	C15	C110	-122.3(4)	.	.	.	no
C115	Ti1	C15	C11	-105.6(2)	.	.	.	no
C115	Ti1	C15	C14	140.5(2)	.	.	.	no
C115	Ti1	C15	C110	18.2(4)	.	.	.	no
C116	Ti1	C15	C11	-101.1(2)	.	.	.	no
C116	Ti1	C15	C14	144.97(19)	.	.	.	no
C116	Ti1	C15	C110	22.7(3)	.	.	.	no
C117	Ti1	C15	C11	-70.9(2)	.	.	.	no
C117	Ti1	C15	C14	175.2(2)	.	.	.	no
C117	Ti1	C15	C110	53.0(3)	.	.	.	no
C118	Ti1	C15	C11	-40.3(2)	.	.	.	no
C118	Ti1	C15	C14	-154.19(19)	.	.	.	no
C118	Ti1	C15	C110	83.6(3)	.	.	.	no
C119	Ti1	C15	C11	-41.1(3)	.	.	.	no
C119	Ti1	C15	C14	-155.1(2)	.	.	.	no
C119	Ti1	C15	C110	82.7(4)	.	.	.	no

O1	Ti1	C115	C116	104.12(19)	.	.	.	.	no
O1	Ti1	C115	C119	-138.43(18)	.	.	.	.	no
C11	Ti1	C115	C116	-45.8(3)	.	.	.	.	no
C11	Ti1	C115	C119	71.7(2)	.	.	.	.	no
C12	Ti1	C115	C116	-100.0(2)	.	.	.	.	no
C12	Ti1	C115	C119	17.5(3)	.	.	.	.	no
C14	Ti1	C115	C116	71.3(4)	.	.	.	.	no
C14	Ti1	C115	C119	-171.3(3)	.	.	.	.	no
C15	Ti1	C115	C116	7.7(3)	.	.	.	.	no
C15	Ti1	C115	C119	125.1(2)	.	.	.	.	no
C116	Ti1	C115	C119	117.5(3)	.	.	.	.	no
C117	Ti1	C115	C116	-34.97(18)	.	.	.	.	no
C117	Ti1	C115	C119	82.48(19)	.	.	.	.	no
C118	Ti1	C115	C116	-75.8(2)	.	.	.	.	no
C118	Ti1	C115	C119	41.63(17)	.	.	.	.	no
C119	Ti1	C115	C116	-117.5(3)	.	.	.	.	no
O1	Ti1	C116	C115	-72.49(19)	.	.	.	.	no
O1	Ti1	C116	C117	168.45(19)	.	.	.	.	no
C11	Ti1	C116	C115	148.63(18)	.	.	.	.	no
C11	Ti1	C116	C117	29.6(2)	.	.	.	.	no
C12	Ti1	C116	C115	125.9(2)	.	.	.	.	no
C12	Ti1	C116	C117	6.8(3)	.	.	.	.	no
C14	Ti1	C116	C115	-148.1(2)	.	.	.	.	no
C14	Ti1	C116	C117	92.9(2)	.	.	.	.	no
C15	Ti1	C116	C115	-174.89(19)	.	.	.	.	no
C15	Ti1	C116	C117	66.0(2)	.	.	.	.	no
C115	Ti1	C116	C117	-119.1(3)	.	.	.	.	no
C117	Ti1	C116	C115	119.1(3)	.	.	.	.	no
C118	Ti1	C116	C115	82.9(2)	.	.	.	.	no
C118	Ti1	C116	C117	-36.19(19)	.	.	.	.	no
C119	Ti1	C116	C115	38.57(19)	.	.	.	.	no
C119	Ti1	C116	C117	-80.5(2)	.	.	.	.	no
O1	Ti1	C117	C116	-13.6(2)	.	.	.	.	no
O1	Ti1	C117	C118	-132.47(17)	.	.	.	.	no
C11	Ti1	C117	C116	-151.9(2)	.	.	.	.	no
C11	Ti1	C117	C118	89.27(19)	.	.	.	.	no
C12	Ti1	C117	C116	-175.32(18)	.	.	.	.	no
C12	Ti1	C117	C118	65.83(19)	.	.	.	.	no
C13	Ti1	C117	C116	-160.01(19)	.	.	.	.	no
C13	Ti1	C117	C118	81.2(2)	.	.	.	.	no
C14	Ti1	C117	C116	-115.4(2)	.	.	.	.	no
C14	Ti1	C117	C118	125.80(19)	.	.	.	.	no
C15	Ti1	C117	C116	-118.7(2)	.	.	.	.	no
C15	Ti1	C117	C118	122.41(19)	.	.	.	.	no
C115	Ti1	C117	C116	35.60(18)	.	.	.	.	no
C115	Ti1	C117	C118	-83.2(2)	.	.	.	.	no
C116	Ti1	C117	C118	-118.9(3)	.	.	.	.	no
C118	Ti1	C117	C116	118.9(3)	.	.	.	.	no
C119	Ti1	C117	C116	79.6(2)	.	.	.	.	no
C119	Ti1	C117	C118	-39.24(18)	.	.	.	.	no
O1	Ti1	C118	C117	74.7(2)	.	.	.	.	no
O1	Ti1	C118	C119	-41.4(2)	.	.	.	.	no
C11	Ti1	C118	C117	-84.98(19)	.	.	.	.	no
C11	Ti1	C118	C119	158.89(17)	.	.	.	.	no
C12	Ti1	C118	C117	-118.17(19)	.	.	.	.	no
C12	Ti1	C118	C119	125.69(16)	.	.	.	.	no
C13	Ti1	C118	C117	-126.59(19)	.	.	.	.	no
C13	Ti1	C118	C119	117.28(17)	.	.	.	.	no
C14	Ti1	C118	C117	-85.5(2)	.	.	.	.	no
C14	Ti1	C118	C119	158.39(18)	.	.	.	.	no
C15	Ti1	C118	C117	-63.1(2)	.	.	.	.	no

C15	Ti1	C118	C119	-179.23(16)	.	.	.	.	no
C115	Ti1	C118	C117	74.79(19)	.	.	.	.	no
C115	Ti1	C118	C119	-41.35(16)	.	.	.	.	no
C116	Ti1	C118	C117	34.83(18)	.	.	.	.	no
C116	Ti1	C118	C119	-81.30(17)	.	.	.	.	no
C117	Ti1	C118	C119	-116.1(2)	.	.	.	.	no
C119	Ti1	C118	C117	116.1(2)	.	.	.	.	no
O1	Ti1	C119	C115	43.20(18)	.	.	.	.	no
O1	Ti1	C119	C118	153.16(15)	.	.	.	.	no
O1	Ti1	C119	C120	-81.43(19)	.	.	.	.	no
C11	Ti1	C119	C115	-133.45(18)	.	.	.	.	no
C11	Ti1	C119	C118	-23.49(19)	.	.	.	.	no
C11	Ti1	C119	C120	101.9(2)	.	.	.	.	no
C12	Ti1	C119	C115	-169.91(17)	.	.	.	.	no
C12	Ti1	C119	C118	-59.95(17)	.	.	.	.	no
C12	Ti1	C119	C120	65.5(2)	.	.	.	.	no
C13	Ti1	C119	C115	158.19(18)	.	.	.	.	no
C13	Ti1	C119	C118	-91.9(2)	.	.	.	.	no
C13	Ti1	C119	C120	33.6(3)	.	.	.	.	no
C15	Ti1	C119	C115	-108.6(2)	.	.	.	.	no
C15	Ti1	C119	C118	1.3(3)	.	.	.	.	no
C15	Ti1	C119	C120	126.7(2)	.	.	.	.	no
C115	Ti1	C119	C118	110.0(2)	.	.	.	.	no
C115	Ti1	C119	C120	-124.6(3)	.	.	.	.	no
C116	Ti1	C119	C115	-35.04(17)	.	.	.	.	no
C116	Ti1	C119	C118	74.92(17)	.	.	.	.	no
C116	Ti1	C119	C120	-159.7(2)	.	.	.	.	no
C117	Ti1	C119	C115	-73.83(18)	.	.	.	.	no
C117	Ti1	C119	C118	36.13(15)	.	.	.	.	no
C117	Ti1	C119	C120	161.5(2)	.	.	.	.	no
C118	Ti1	C119	C115	-110.0(2)	.	.	.	.	no
C118	Ti1	C119	C120	125.4(3)	.	.	.	.	no
Ti1	O1	C114	C113	-160.7(2)	.	.	.	.	no
C111	O1	C114	C113	22.2(4)	.	.	.	.	no
Ti1	O1	C111	C112	177.3(2)	.	.	.	.	no
C114	O1	C111	C112	-5.9(4)	.	.	.	.	no
C34	O3	C31	C32	-22.2(6)	.	.	.	.	no
C31	O3	C34	C33	29.3(6)	.	.	.	.	no
C42	O4	C41	C43	-15.9(18)	.	.	.	.	no
C41	O4	C42	C44	40(2)	.	.	.	.	no
Ti1	C11	C15	C110	-121.2(4)	.	.	.	.	no
C15	C11	C12	C13	-1.8(4)	.	.	.	.	no
C15	C11	C12	C17	-168.7(3)	.	.	.	.	no
C16	C11	C12	Ti1	-127.2(3)	.	.	.	.	no
C16	C11	C12	C13	169.2(3)	.	.	.	.	no
C16	C11	C15	C110	3.5(6)	.	.	.	.	no
Ti1	C11	C12	C13	-63.7(2)	.	.	.	.	no
Ti1	C11	C12	C17	129.5(3)	.	.	.	.	no
C15	C11	C12	Ti1	61.8(2)	.	.	.	.	no
Ti1	C11	C15	C14	67.5(3)	.	.	.	.	no
C12	C11	C15	Ti1	-64.5(3)	.	.	.	.	no
C12	C11	C15	C14	3.1(4)	.	.	.	.	no
C16	C11	C12	C17	2.4(5)	.	.	.	.	no
C12	C11	C15	C110	174.3(4)	.	.	.	.	no
C16	C11	C15	C14	-167.7(3)	.	.	.	.	no
C16	C11	C15	Ti1	124.7(4)	.	.	.	.	no
C17	C12	C13	C18	-5.6(6)	.	.	.	.	no
C17	C12	C13	C14	166.3(3)	.	.	.	.	no
C11	C12	C13	C18	-172.0(4)	.	.	.	.	no
C17	C12	C13	Ti1	-130.0(3)	.	.	.	.	no
C11	C12	C13	C14	-0.1(4)	.	.	.	.	no

Ti1	C12	C13	C18	124.4(4)	.	.	.	.	no
Ti1	C12	C13	C14	-63.7(3)	.	.	.	.	no
C11	C12	C13	Ti1	63.6(2)	.	.	.	.	no
Ti1	C13	C14	C15	-63.1(3)	.	.	.	.	no
C18	C13	C14	C19	1.5(6)	.	.	.	.	no
Ti1	C13	C14	C19	124.5(4)	.	.	.	.	no
C12	C13	C14	Ti1	65.1(2)	.	.	.	.	no
C18	C13	C14	Ti1	-123.0(4)	.	.	.	.	no
C18	C13	C14	C15	173.9(4)	.	.	.	.	no
C12	C13	C14	C15	2.0(4)	.	.	.	.	no
C12	C13	C14	C19	-170.4(4)	.	.	.	.	no
C19	C14	C15	Ti1	-122.3(4)	.	.	.	.	no
C13	C14	C15	C110	-174.5(4)	.	.	.	.	no
C19	C14	C15	C11	169.3(4)	.	.	.	.	no
C13	C14	C15	C11	-3.2(4)	.	.	.	.	no
C19	C14	C15	C110	-2.0(6)	.	.	.	.	no
Ti1	C14	C15	C110	120.3(4)	.	.	.	.	no
Ti1	C14	C15	C11	-68.4(3)	.	.	.	.	no
C13	C14	C15	Ti1	65.3(3)	.	.	.	.	no
O1	C111	C112	H112	-132.62	.	.	.	.	no
O1	C111	C112	H112'	107.25	.	.	.	.	no
H111	C111	C112	H112	-12.53	.	.	.	.	no
H111'	C111	C112	H112'	-12.70	.	.	.	.	no
H111'	C111	C112	C113	-132.61	.	.	.	.	no
H111	C111	C112	H112'	-132.67	.	.	.	.	no
H111	C111	C112	C113	107.43	.	.	.	.	no
H111'	C111	C112	H112	107.43	.	.	.	.	no
C111	C112	C113	H113'	-93.36	.	.	.	.	no
H112'	C112	C113	C114	-93.91	.	.	.	.	no
C111	C112	C113	H113	145.47	.	.	.	.	no
H112	C112	C113	H113'	26.62	.	.	.	.	no
H112	C112	C113	H113	-94.55	.	.	.	.	no
H112	C112	C113	C114	146.03	.	.	.	.	no
H112'	C112	C113	H113	25.51	.	.	.	.	no
H112'	C112	C113	H113'	146.67	.	.	.	.	no
H113	C113	C114	H114'	91.59	.	.	.	.	no
H113'	C113	C114	O1	90.11	.	.	.	.	no
H113	C113	C114	H114	-29.09	.	.	.	.	no
H113'	C113	C114	H114'	-29.56	.	.	.	.	no
C112	C113	C114	H114	90.35	.	.	.	.	no
H113'	C113	C114	H114	-150.24	.	.	.	.	no
H113	C113	C114	O1	-148.74	.	.	.	.	no
C112	C113	C114	H114'	-148.97	.	.	.	.	no
H115	C115	C119	C120	-34.22	.	.	.	.	no
H115	C115	C116	C117	-179.02	.	.	.	.	no
H115	C115	C116	Ti1	120.16	.	.	.	.	no
C119	C115	C116	H116	-179.03	.	.	.	.	no
H115	C115	C119	C118	178.18	.	.	.	.	no
H115	C115	C116	H116	0.95	.	.	.	.	no
Ti1	C115	C116	H116	-119.21	.	.	.	.	no
H115	C115	C119	Ti1	-112.56	.	.	.	.	no
C115	C116	C117	H117	-179.68	.	.	.	.	no
H116	C116	C117	H117	0.35	.	.	.	.	no
H116	C116	C117	C118	-179.69	.	.	.	.	no
H116	C116	C117	Ti1	122.06	.	.	.	.	no
Ti1	C116	C117	H117	-121.70	.	.	.	.	no
H117	C117	C118	H118	-1.46	.	.	.	.	no
H117	C117	C118	C119	178.50	.	.	.	.	no
C116	C117	C118	H118	178.58	.	.	.	.	no
H117	C117	C118	Ti1	116.81	.	.	.	.	no
Ti1	C117	C118	H118	-118.27	.	.	.	.	no

H118	C118	C119	Ti1	111.48	.	.	.	.	no
H118	C118	C119	C120	34.51	.	.	.	.	no
H118	C118	C119	C115	-178.05	.	.	.	.	no
C121	C120	C125	H125	177.28	.	.	.	.	no
C119	C120	C125	H125	-39.19	.	.	.	.	no
C125	C120	C121	H121	-177.29	.	.	.	.	no
C119	C120	C121	H121	39.20	.	.	.	.	no
C122	C121	C126	H126'	179.16	.	.	.	.	no
H121	C121	C122	H122	-59.19	.	.	.	.	no
C120	C121	C126	H126'	-63.02	.	.	.	.	no
C120	C121	C126	H126	178.49	.	.	.	.	no
C26	C21	B2	C219	-163.9(3)	.	.	.	.	no
C122	C121	C126	H126	60.67	.	.	.	.	no
H121	C121	C126	C127	179.98	.	.	.	.	no
H121	C121	C122	H122'	59.29	.	.	.	.	no
H121	C121	C122	C123	-179.96	.	.	.	.	no
C126	C121	C122	H122'	-60.62	.	.	.	.	no
C126	C121	C122	H122	-179.11	.	.	.	.	no
C26	C21	B2	C213	-42.4(4)	.	.	.	.	no
C26	C21	C22	C23	-0.1(4)	.	.	.	.	no
B2	C21	C22	C23	179.7(3)	.	.	.	.	no
C22	C21	C26	C25	0.2(5)	.	.	.	.	no
H121	C121	C126	H126'	59.22	.	.	.	.	no
H121	C121	C126	H126	-59.27	.	.	.	.	no
C26	C21	B2	C27	75.8(3)	.	.	.	.	no
C22	C21	B2	C213	137.8(3)	.	.	.	.	no
C22	C21	B2	C219	16.4(4)	.	.	.	.	no
C120	C121	C122	H122'	178.77	.	.	.	.	no
C120	C121	C122	H122	60.28	.	.	.	.	no
C22	C21	B2	C27	-103.9(3)	.	.	.	.	no
B2	C21	C26	C25	-179.5(3)	.	.	.	.	no
H122'	C122	C123	H123	-59.43	.	.	.	.	no
H122	C122	C123	C128	179.28	.	.	.	.	no
C121	C122	C123	H123	179.82	.	.	.	.	no
H122	C122	C123	C124	-61.71	.	.	.	.	no
H122'	C122	C123	C124	179.80	.	.	.	.	no
H122'	C122	C123	C128	60.78	.	.	.	.	no
C21	C22	C23	C24	-0.2(5)	.	.	.	.	no
H122	C122	C123	H123	59.07	.	.	.	.	no
C128	C123	C124	H124	-60.15	.	.	.	.	no
H123	C123	C128	H128	-59.97	.	.	.	.	no
C128	C123	C124	H124'	-179.01	.	.	.	.	no
C122	C123	C124	H124	-179.09	.	.	.	.	no
H123	C123	C124	H124'	-58.72	.	.	.	.	no
C124	C123	C128	H128	60.32	.	.	.	.	no
H123	C123	C124	C125	-179.29	.	.	.	.	no
C122	C123	C124	H124'	62.05	.	.	.	.	no
H123	C123	C124	H124	60.14	.	.	.	.	no
C122	C123	C128	H128	179.84	.	.	.	.	no
C124	C123	C128	H128'	178.96	.	.	.	.	no
C122	C123	C128	H128'	-61.51	.	.	.	.	no
H123	C123	C128	H128'	58.68	.	.	.	.	no
H123	C123	C128	C127	179.34	.	.	.	.	no
C22	C23	C24	C25	0.4(5)	.	.	.	.	no
H124	C124	C125	C129	60.07	.	.	.	.	no
H124'	C124	C125	C129	179.07	.	.	.	.	no
C123	C124	C125	H125	179.46	.	.	.	.	no
H124	C124	C125	C120	-178.97	.	.	.	.	no
H124'	C124	C125	H125	58.96	.	.	.	.	no
H124	C124	C125	H125	-60.04	.	.	.	.	no
C23	C24	C25	C26	-0.3(5)	.	.	.	.	no

H124'	C124	C125	C120	-59.97	.	.	.	no
H125	C125	C129	H129'	58.52	.	.	.	no
C120	C125	C129	H129'	179.20	.	.	.	no
H125	C125	C129	C127	179.03	.	.	.	no
C124	C125	C129	H129	179.43	.	.	.	no
C124	C125	C129	H129'	-61.54	.	.	.	no
H125	C125	C129	H129	-60.51	.	.	.	no
C24	C25	C26	C21	-0.1(5)	.	.	.	no
C120	C125	C129	H129	60.16	.	.	.	no
C121	C126	C127	H127	-179.50	.	.	.	no
H126	C126	C127	H127	59.74	.	.	.	no
H126	C126	C127	C128	-60.27	.	.	.	no
H126'	C126	C127	C129	60.72	.	.	.	no
H126	C126	C127	C129	179.20	.	.	.	no
H126'	C126	C127	C128	-178.76	.	.	.	no
H126'	C126	C127	H127	-58.74	.	.	.	no
C126	C127	C128	H128	179.71	.	.	.	no
C126	C127	C128	H128'	60.98	.	.	.	no
C126	C127	C129	H129'	-178.16	.	.	.	no
B2	C27	C28	C29	-172.9(3)	.	.	.	no
C129	C127	C128	H128'	-179.51	.	.	.	no
C28	C27	B2	C213	90.4(3)	.	.	.	no
C28	C27	B2	C219	-149.8(3)	.	.	.	no
C28	C27	B2	C21	-27.2(4)	.	.	.	no
H127	C127	C129	H129	60.29	.	.	.	no
H127	C127	C128	H128	59.68	.	.	.	no
C212	C27	B2	C219	36.4(4)	.	.	.	no
H127	C127	C128	H128'	-59.05	.	.	.	no
C212	C27	B2	C213	-83.4(3)	.	.	.	no
C126	C127	C129	H129	-59.16	.	.	.	no
C212	C27	B2	C21	159.1(3)	.	.	.	no
C129	C127	C128	H128	-60.78	.	.	.	no
C212	C27	C28	C29	1.2(4)	.	.	.	no
H127	C127	C129	C125	-179.23	.	.	.	no
H127	C127	C129	H129'	-58.71	.	.	.	no
H127	C127	C128	C123	-179.66	.	.	.	no
C28	C27	C212	C211	-1.0(4)	.	.	.	no
C128	C127	C129	H129'	61.72	.	.	.	no
C128	C127	C129	H129	-179.28	.	.	.	no
B2	C27	C212	C211	173.3(3)	.	.	.	no
C27	C28	C29	C210	-0.2(4)	.	.	.	no
C28	C29	C210	C211	-1.0(4)	.	.	.	no
C29	C210	C211	C212	1.2(5)	.	.	.	no
C210	C211	C212	C27	-0.1(5)	.	.	.	no
C218	C213	B2	C27	-168.9(2)	.	.	.	no
C214	C213	B2	C219	-106.7(3)	.	.	.	no
C218	C213	B2	C21	-48.7(3)	.	.	.	no
C218	C213	C214	C215	0.6(4)	.	.	.	no
C214	C213	B2	C21	131.2(3)	.	.	.	no
B2	C213	C218	C217	178.9(3)	.	.	.	no
C218	C213	B2	C219	73.4(3)	.	.	.	no
C214	C213	B2	C27	11.0(4)	.	.	.	no
C214	C213	C218	C217	-1.0(4)	.	.	.	no
B2	C213	C214	C215	-179.3(3)	.	.	.	no
C213	C214	C215	C216	0.0(5)	.	.	.	no
C214	C215	C216	C217	-0.3(5)	.	.	.	no
C215	C216	C217	C218	0.0(5)	.	.	.	no
C216	C217	C218	C213	0.7(5)	.	.	.	no
C224	C219	B2	C213	173.5(2)	.	.	.	no
C224	C219	C220	C221	0.4(4)	.	.	.	no
C224	C219	B2	C27	55.2(3)	.	.	.	no

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 C220    C219    C224    C223        -1.0(4)     .       .       .       .   no
 C220    C219    B2      C213        -3.5(4)     .       .       .       .   no
 B2      C219    C220    C221       177.5(3)     .       .       .       .   no
 C224    C219    B2      C21        -67.2(3)     .       .       .       .   no
 C220    C219    B2      C21        115.9(3)     .       .       .       .   no
 B2      C219    C224    C223      -178.2(3)     .       .       .       .   no
 C220    C219    B2      C27       -121.7(3)     .       .       .       .   no
 C219    C220    C221    C222         0.5(5)     .       .       .       .   no
 C220    C221    C222    C223        -0.9(5)     .       .       .       .   no
 C221    C222    C223    C224         0.3(5)     .       .       .       .   no
 C222    C223    C224    C219         0.7(5)     .       .       .       .   no
 C53     C51     C52     C53          -73(3)     .       .       .   3_666 no
 C52     C51     C53     C52           77(3)     .       .       .   3_666 no
 C51     C52     C53     C51           75(3)     .       .   3_666   3_666 no
 O3      C31     C32     C33          5.9(7)     .       .       .       .   no
 C31     C32     C33     C34         11.7(7)     .       .       .       .   no
 C32     C33     C34     O3         -25.6(7)     .       .       .       .   no
 O4      C41     C43     C44       -13.3(17)     .       .       .       .   no
 O4      C42     C44     C43          -50(2)     .       .       .       .   no
 C41     C43     C44     C42        38.1(18)     .       .       .       .   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
 Ti1     C121       3.655(3)                    .       .                   no
 Ti1     C125       3.530(4)                    .       .                   no
 Ti1     H121         3.6031                    .       .                   no
 Ti1     H125         3.3817                    .       .                   no
 O1      C13        3.386(4)                    .       .                   no
 O1      C14        2.916(4)                    .       .                   no
 O1      C19        3.069(5)                    .       .                   no
 O1      C115       2.844(3)                    .       .                   no
 O1      C116       3.223(3)                    .       .                   no
 O1      H19"         2.8147                    .       .                   no
 O1      H115         2.7686                    .       .                   no
 O3      H29          2.8206                    .   1_655                   no
 C11     C14        2.300(5)                    .       .                   no
 C11     C17        2.580(5)                    .       .                   no
 C11     C110       2.618(5)                    .       .                   no
 C11     C117       3.108(4)                    .       .                   no
 C11     C118       3.055(4)                    .       .                   no
 C11     C13        2.306(5)                    .       .                   no
 C12     C118       3.302(4)                    .       .                   no
 C12     C16        2.591(5)                    .       .                   no
 C12     C14        2.303(4)                    .       .                   no
 C12     C15        2.297(5)                    .       .                   no
 C12     C18        2.623(5)                    .       .                   no
 C13     C11        2.306(5)                    .       .                   no
 C13     C15        2.308(5)                    .       .                   no
 C13     O1         3.386(4)                    .       .                   no
 C13     C19        2.618(5)                    .       .                   no
 C13     C17        2.627(5)                    .       .                   no
 C14     C12        2.303(4)                    .       .                   no
 C14     C110       2.612(6)                    .       .                   no
 C14     O1         2.916(4)                    .       .                   no
 C14     C11        2.300(5)                    .       .                   no
 C14     C18        2.618(5)                    .       .                   no
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C15	C117	3.396(4)	.	.	no
C15	C16	2.619(5)	.	.	no
C15	C12	2.297(5)	.	.	no
C15	C13	2.308(5)	.	.	no
C15	C19	2.609(5)	.	.	no
C17	C121	3.496(5)	.	.	no
C17	C126	3.579(5)	.	.	no
C19	C28	3.578(5)	.	4_555	no
C19	C111	3.443(6)	.	.	no
C22	C224	3.268(4)	.	.	no
C22	C114	3.590(5)	.	4_554	no
C26	C28	3.338(4)	.	.	no
C26	C218	3.288(4)	.	.	no
C28	C19	3.578(5)	.	4_454	no
C28	C26	3.338(4)	.	.	no
C11	H51	2.9565	.	.	no
C11	H117	3.0768	.	.	no
C11	H118	2.9984	.	.	no
C111	C19	3.443(6)	.	.	no
C114	C22	3.590(5)	.	4_455	no
C115	C117	2.263(5)	.	.	no
C115	C114	3.279(5)	.	.	no
C115	C120	2.519(4)	.	.	no
C115	C118	2.283(4)	.	.	no
C115	O1	2.844(3)	.	.	no
C16	H17	2.8881	.	.	no
C16	H41	3.0057	.	1_455	no
C116	O1	3.223(3)	.	.	no
C116	C118	2.281(4)	.	.	no
C116	C119	2.325(4)	.	.	no
C16	H110'	2.9188	.	.	no
C116	C114	3.292(5)	.	.	no
C16	H117	2.8340	.	.	no
C16	H51	2.9173	.	.	no
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C17	H18'	2.9415	.	.	no
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C17	H121	2.8264	.	.	no
C17	H224	2.8920	.	.	no
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C111	H19'	2.9292	.	.	no
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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Cl1 Cl 0.35448(4) 0.04525(4) 0.16503(3) 0.03995(13) Uani 1 1 d . . .
C1 C 0.39649(15) 0.09825(15) 0.40748(12) 0.0252(4) Uani 1 1 d . . .
C2 C 0.38293(16) 0.22208(15) 0.46310(13) 0.0288(4) Uani 1 1 d . . .
H2 H 0.3286(18) 0.2515(17) 0.5127(14) 0.035 Uiso 1 1 d . . .
C3 C 0.45149(17) 0.29239(17) 0.43082(15) 0.0370(5) Uani 1 1 d . . .
H3 H 0.456(2) 0.374(2) 0.4523(15) 0.044 Uiso 1 1 d . . .
C4 C 0.51020(17) 0.21863(19) 0.35807(17) 0.0394(5) Uani 1 1 d . . .
H4 H 0.563(2) 0.243(2) 0.3211(16) 0.047 Uiso 1 1 d . . .
C5 C 0.48014(16) 0.10014(18) 0.34461(15) 0.0322(4) Uani 1 1 d . . .
H5 H 0.5041(19) 0.0330(19) 0.2995(15) 0.039 Uiso 1 1 d . . .
C6 C 0.30584(14) 0.00798(14) 0.38291(11) 0.0220(3) Uani 1 1 d . . .
C7 C 0.32561(16) -0.11704(15) 0.31555(12) 0.0264(4) Uani 1 1 d . . .
H7 H 0.3729(18) -0.1111(17) 0.2673(14) 0.032 Uiso 1 1 d . . .
C8 C 0.21383(17) -0.18918(16) 0.27399(13) 0.0308(4) Uani 1 1 d . . .
H8A H 0.1755(18) -0.1519(18) 0.2383(14) 0.037 Uiso 1 1 d . . .
H8B H 0.2315(18) -0.2666(19) 0.2313(15) 0.037 Uiso 1 1 d . . .
C9 C 0.14190(17) -0.19724(15) 0.34999(13) 0.0299(4) Uani 1 1 d . . .
H9 H 0.074(2) -0.2412(18) 0.3231(15) 0.036 Uiso 1 1 d . . .
C10 C 0.11892(16) -0.07181(15) 0.41457(13) 0.0287(4) Uani 1 1 d . . .
H10A H 0.0738(18) -0.0768(17) 0.4645(15) 0.034 Uiso 1 1 d . . .
H10B H 0.0786(18) -0.0343(17) 0.3813(14) 0.034 Uiso 1 1 d . . .
C11 C 0.23012(15) 0.00172(14) 0.45657(11) 0.0233(4) Uani 1 1 d . . .
H11 H 0.2117(17) 0.0813(17) 0.4996(13) 0.028 Uiso 1 1 d . . .
C12 C 0.29285(18) -0.05944(16) 0.51089(13) 0.0295(4) Uani 1 1 d . . .
H12A H 0.360(2) -0.0140(18) 0.5402(15) 0.035 Uiso 1 1 d . . .
H12B H 0.2464(19) -0.0615(18) 0.5593(15) 0.035 Uiso 1 1 d . . .
C13 C 0.31653(16) -0.18488(15) 0.44623(13) 0.0295(4) Uani 1 1 d . . .
H13 H 0.3565(18) -0.2245(18) 0.4791(14) 0.035 Uiso 1 1 d . . .
C14 C 0.38859(17) -0.17846(17) 0.36965(14) 0.0310(4) Uani 1 1 d . . .
H14A H 0.461(2) -0.1330(18) 0.3948(15) 0.037 Uiso 1 1 d . . .
H14B H 0.4055(18) -0.2600(19) 0.3274(14) 0.037 Uiso 1 1 d . . .
C15 C 0.20503(17) -0.25727(16) 0.40394(14) 0.0321(4) Uani 1 1 d . . .
H15A H 0.1579(19) -0.2646(18) 0.4518(15) 0.039 Uiso 1 1 d . . .
H15B H 0.2203(18) -0.3405(19) 0.3613(15) 0.039 Uiso 1 1 d . . .
C16 C 0.17060(15) 0.21595(14) 0.22763(11) 0.0229(4) Uani 1 1 d . . .
C17 C 0.23510(15) 0.32141(14) 0.28537(11) 0.0235(4) Uani 1 1 d . . .
C18 C 0.21223(15) 0.34189(14) 0.37725(11) 0.0229(4) Uani 1 1 d . . .
C19 C 0.13835(14) 0.24666(14) 0.37645(11) 0.0212(3) Uani 1 1 d . . .
C20 C 0.11299(14) 0.16830(14) 0.28324(11) 0.0211(3) Uani 1 1 d . . .
C21 C 0.1535(2) 0.17068(19) 0.12496(13) 0.0370(5) Uani 1 1 d . . .
H21A H 0.138(2) 0.080(2) 0.0968(16) 0.044 Uiso 1 1 d . . .
H21B H 0.095(2) 0.2102(19) 0.1093(15) 0.044 Uiso 1 1 d . . .
H21C H 0.221(2) 0.1917(19) 0.1009(16) 0.044 Uiso 1 1 d . . .
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C22 C 0.3065(2) 0.40054(19) 0.25265(17) 0.0385(5) Uani 1 1 d . . .
H22A H 0.263(2) 0.457(2) 0.2381(15) 0.046 Uiso 1 1 d . . .
H22B H 0.359(2) 0.446(2) 0.2987(17) 0.046 Uiso 1 1 d . . .
H22C H 0.344(2) 0.359(2) 0.2001(17) 0.046 Uiso 1 1 d . . .
C23 C 0.2452(2) 0.45406(17) 0.45999(14) 0.0372(5) Uani 1 1 d . . .
H23A H 0.264(2) 0.4381(19) 0.5123(17) 0.045 Uiso 1 1 d . . .
H23B H 0.181(2) 0.508(2) 0.4738(15) 0.045 Uiso 1 1 d . . .
H23C H 0.308(2) 0.501(2) 0.4465(16) 0.045 Uiso 1 1 d . . .
C24 C 0.08173(19) 0.24437(18) 0.45912(13) 0.0319(4) Uani 1 1 d . . .
H24A H 0.046(2) 0.172(2) 0.4478(15) 0.038 Uiso 1 1 d . . .
H24B H 0.1354(19) 0.2706(18) 0.5131(15) 0.038 Uiso 1 1 d . . .
H24C H 0.0224(19) 0.2985(19) 0.4744(14) 0.038 Uiso 1 1 d . . .
C25 C 0.02957(17) 0.06208(16) 0.24622(15) 0.0318(4) Uani 1 1 d . . .
H25A H -0.0108(19) 0.0520(18) 0.2942(16) 0.038 Uiso 1 1 d . . .
H25B H -0.026(2) 0.0693(18) 0.2071(15) 0.038 Uiso 1 1 d . . .
H25C H 0.0646(19) -0.0107(19) 0.2135(15) 0.038 Uiso 1 1 d . . .
Ti2 Ti 0.72052(2) 0.37933(2) 0.151618(18) 0.01728(8) Uani 1 1 d . . .
Cl2 Cl 0.64173(4) 0.44572(4) 0.29594(3) 0.02709(10) Uani 1 1 d . . .
C26 C 0.63584(14) 0.47102(14) 0.07805(11) 0.0213(3) Uani 1 1 d . . .
C27 C 0.68466(17) 0.37405(15) 0.00744(11) 0.0280(4) Uani 1 1 d . . .
H27 H 0.7469(19) 0.3836(18) -0.0232(15) 0.034 Uiso 1 1 d . . .
C28 C 0.62725(18) 0.26701(16) 0.00029(13) 0.0353(5) Uani 1 1 d . . .
H28 H 0.6413(19) 0.190(2) -0.0402(15) 0.042 Uiso 1 1 d . . .
C29 C 0.54327(18) 0.29266(16) 0.06299(14) 0.0347(5) Uani 1 1 d . . .
H29 H 0.495(2) 0.237(2) 0.0728(15) 0.042 Uiso 1 1 d . . .
C30 C 0.54506(15) 0.41662(15) 0.10830(13) 0.0268(4) Uani 1 1 d . . .
H30 H 0.4997(18) 0.4566(17) 0.1557(14) 0.032 Uiso 1 1 d . . .
C31 C 0.70315(14) 0.57375(13) 0.14010(10) 0.0184(3) Uani 1 1 d . . .
C32 C 0.79414(15) 0.63398(15) 0.10559(12) 0.0235(4) Uani 1 1 d . . .
H32 H 0.8357(17) 0.5780(17) 0.0590(14) 0.028 Uiso 1 1 d . . .
C33 C 0.73736(18) 0.71242(17) 0.06271(13) 0.0301(4) Uani 1 1 d . . .
H33A H 0.7931(19) 0.7538(18) 0.0401(14) 0.036 Uiso 1 1 d . . .
H33B H 0.6866(19) 0.6636(18) 0.0130(15) 0.036 Uiso 1 1 d . . .
C34 C 0.67342(16) 0.80501(15) 0.13606(13) 0.0282(4) Uani 1 1 d . . .
H34 H 0.6379(18) 0.8533(17) 0.1101(14) 0.034 Uiso 1 1 d . . .
C35 C 0.58504(16) 0.74266(15) 0.17294(13) 0.0258(4) Uani 1 1 d . . .
H35A H 0.5430(17) 0.8030(17) 0.2195(14) 0.031 Uiso 1 1 d . . .
H35B H 0.5325(18) 0.6955(17) 0.1251(14) 0.031 Uiso 1 1 d . . .
C36 C 0.64252(15) 0.66565(13) 0.21609(11) 0.0198(3) Uani 1 1 d . . .
H36 H 0.5890(17) 0.6291(16) 0.2419(13) 0.024 Uiso 1 1 d . . .
C37 C 0.72594(16) 0.74461(15) 0.29471(12) 0.0262(4) Uani 1 1 d . . .
H37A H 0.7610(17) 0.6979(17) 0.3231(14) 0.031 Uiso 1 1 d . . .
H37B H 0.6848(17) 0.8026(17) 0.3429(14) 0.031 Uiso 1 1 d . . .
C38 C 0.81437(17) 0.80751(15) 0.25836(13) 0.0297(4) Uani 1 1 d . . .
H38 H 0.8690(18) 0.8596(17) 0.3103(14) 0.036 Uiso 1 1 d . . .
C39 C 0.87643(16) 0.71371(17) 0.18546(13) 0.0294(4) Uani 1 1 d . . .
H39A H 0.9346(19) 0.7536(18) 0.1643(14) 0.035 Uiso 1 1 d . . .
H39B H 0.9107(18) 0.6672(18) 0.2135(14) 0.035 Uiso 1 1 d . . .
C40 C 0.75666(19) 0.88391(16) 0.21526(15) 0.0341(4) Uani 1 1 d . . .
H40A H 0.7137(19) 0.943(2) 0.2623(15) 0.041 Uiso 1 1 d . . .
H40B H 0.813(2) 0.9261(19) 0.1929(15) 0.041 Uiso 1 1 d . . .
C41 C 0.92473(14) 0.37645(15) 0.13949(11) 0.0235(4) Uani 1 1 d . . .
C42 C 0.90387(14) 0.38881(14) 0.23024(11) 0.0216(3) Uani 1 1 d . . .
C43 C 0.83920(14) 0.28532(14) 0.22521(11) 0.0213(3) Uani 1 1 d . . .
C44 C 0.81617(15) 0.21028(14) 0.13095(11) 0.0238(4) Uani 1 1 d . . .
C45 C 0.87113(15) 0.26556(15) 0.07832(11) 0.0247(4) Uani 1 1 d . . .
C46 C 1.00863(18) 0.4499(2) 0.11188(16) 0.0354(4) Uani 1 1 d . . .
H46A H 1.035(2) 0.520(2) 0.1607(16) 0.042 Uiso 1 1 d . . .
H46B H 0.982(2) 0.4727(19) 0.0641(16) 0.042 Uiso 1 1 d . . .
H46C H 1.077(2) 0.4089(19) 0.0908(15) 0.042 Uiso 1 1 d . . .
C47 C 0.95123(18) 0.48681(18) 0.31756(13) 0.0324(4) Uani 1 1 d . . .
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H47A H 1.013(2) 0.4636(18) 0.3440(15) 0.039 Uiso 1 1 d . . .
H47B H 0.9712(19) 0.5582(19) 0.3106(15) 0.039 Uiso 1 1 d . . .
H47C H 0.896(2) 0.5072(19) 0.3591(16) 0.039 Uiso 1 1 d . . .
C48 C 0.81053(18) 0.25725(19) 0.30638(13) 0.0300(4) Uani 1 1 d . . .
H48A H 0.7790(18) 0.3201(19) 0.3536(15) 0.036 Uiso 1 1 d . . .
H48B H 0.8807(19) 0.2470(18) 0.3351(14) 0.036 Uiso 1 1 d . . .
H48C H 0.765(2) 0.190(2) 0.2899(14) 0.036 Uiso 1 1 d . . .
C49 C 0.7560(2) 0.08799(16) 0.09419(15) 0.0366(5) Uani 1 1 d . . .
H49A H 0.721(2) 0.0665(19) 0.0346(17) 0.044 Uiso 1 1 d . . .
H49B H 0.807(2) 0.029(2) 0.0931(15) 0.044 Uiso 1 1 d . . .
H49C H 0.696(2) 0.0846(19) 0.1324(16) 0.044 Uiso 1 1 d . . .
C50 C 0.8902(2) 0.2081(2) -0.02238(13) 0.0385(5) Uani 1 1 d . . .
H50A H 0.900(2) 0.265(2) -0.0474(16) 0.046 Uiso 1 1 d . . .
H50B H 0.831(2) 0.149(2) -0.0538(17) 0.046 Uiso 1 1 d . . .
H50C H 0.957(2) 0.171(2) -0.0311(15) 0.046 Uiso 1 1 d . . .

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Cl1 0.0455(3) 0.0423(3) 0.0287(2) 0.00686(19) 0.0084(2) 0.0235(2)
C1 0.0206(10) 0.0294(8) 0.0320(9) 0.0197(7) -0.0066(7) 0.0011(7)
C2 0.0282(11) 0.0285(9) 0.0312(10) 0.0153(8) -0.0137(8) -0.0026(8)
C3 0.0296(12) 0.0303(10) 0.0542(13) 0.0237(9) -0.0222(9) -0.0099(8)
C4 0.0163(11) 0.0485(12) 0.0686(15) 0.0418(11) -0.0075(9) -0.0071(9)
C5 0.0170(10) 0.0398(10) 0.0501(12) 0.0286(9) -0.0012(8) 0.0046(8)
C6 0.0203(10) 0.0228(8) 0.0254(8) 0.0124(7) -0.0004(6) 0.0028(7)
C7 0.0282(11) 0.0250(8) 0.0300(9) 0.0135(7) 0.0081(7) 0.0089(8)
C8 0.0384(12) 0.0233(8) 0.0274(9) 0.0067(7) -0.0050(8) 0.0044(8)
C9 0.0207(11) 0.0240(8) 0.0426(11) 0.0122(8) -0.0086(8) -0.0048(7)
C10 0.0223(10) 0.0293(9) 0.0384(10) 0.0172(8) 0.0037(8) 0.0046(8)
C11 0.0257(10) 0.0209(8) 0.0244(9) 0.0098(7) 0.0020(7) 0.0032(7)
C12 0.0339(12) 0.0311(9) 0.0267(9) 0.0157(8) -0.0035(8) -0.0014(8)
C13 0.0277(11) 0.0293(9) 0.0385(10) 0.0210(8) -0.0029(8) 0.0048(8)
C14 0.0231(11) 0.0292(9) 0.0458(11) 0.0193(9) 0.0032(8) 0.0075(8)
C15 0.0321(12) 0.0249(9) 0.0438(11) 0.0186(8) 0.0016(8) 0.0001(8)
C16 0.0234(10) 0.0261(8) 0.0210(8) 0.0100(7) 0.0009(6) 0.0112(7)
C17 0.0239(10) 0.0237(8) 0.0272(9) 0.0138(7) 0.0033(7) 0.0079(7)
C18 0.0244(10) 0.0194(7) 0.0226(8) 0.0054(6) -0.0016(7) 0.0059(7)
C19 0.0191(9) 0.0230(8) 0.0223(8) 0.0089(6) 0.0030(6) 0.0073(7)
C20 0.0171(9) 0.0209(7) 0.0244(8) 0.0074(6) -0.0017(6) 0.0064(7)
C21 0.0502(14) 0.0414(11) 0.0220(9) 0.0133(8) -0.0006(8) 0.0188(10)
C22 0.0422(14) 0.0338(10) 0.0483(13) 0.0247(10) 0.0120(10) 0.0059(10)
C23 0.0475(14) 0.0240(9) 0.0313(11) 0.0023(8) -0.0082(9) 0.0018(9)
C24 0.0361(12) 0.0324(10) 0.0297(10) 0.0126(8) 0.0133(8) 0.0110(9)
C25 0.0260(11) 0.0267(9) 0.0401(11) 0.0114(8) -0.0103(8) 0.0016(8)
Ti2 0.01706(17) 0.01748(13) 0.01720(14) 0.00686(11) -0.00188(10) 0.00180(11)
Cl2 0.0278(2) 0.0326(2) 0.0284(2) 0.01852(17) 0.00948(16) 0.00947(18)
C26 0.0210(9) 0.0236(8) 0.0211(8) 0.0106(6) -0.0054(6) 0.0058(7)
C27 0.0345(11) 0.0309(9) 0.0166(8) 0.0065(7) -0.0059(7) 0.0117(8)
C28 0.0424(13) 0.0241(9) 0.0294(10) 0.0010(8) -0.0207(8) 0.0059(8)
C29 0.0280(12) 0.0258(9) 0.0470(12) 0.0136(8) -0.0195(9) -0.0068(8)
C30 0.0194(10) 0.0270(8) 0.0340(10) 0.0130(8) -0.0090(7) 0.0010(7)
C31 0.0188(9) 0.0212(7) 0.0176(8) 0.0097(6) 0.0009(6) 0.0049(7)
C32 0.0208(10) 0.0306(9) 0.0238(8) 0.0151(7) 0.0043(7) 0.0045(8)
C33 0.0311(12) 0.0392(10) 0.0296(10) 0.0243(8) 0.0010(8) -0.0010(9)
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C34 0.0300(11) 0.0259(8) 0.0358(10) 0.0205(8) -0.0061(8) 0.0013(8)
C35 0.0216(10) 0.0249(8) 0.0327(10) 0.0127(7) -0.0009(7) 0.0058(8)
C36 0.0206(10) 0.0188(7) 0.0221(8) 0.0099(6) 0.0046(6) 0.0033(7)
C37 0.0345(11) 0.0229(8) 0.0218(8) 0.0092(7) -0.0017(7) 0.0057(8)
C38 0.0303(11) 0.0248(8) 0.0333(10) 0.0129(8) -0.0115(8) -0.0048(8)
C39 0.0177(10) 0.0375(10) 0.0396(11) 0.0229(9) -0.0014(7) -0.0022(8)
C40 0.0361(12) 0.0251(9) 0.0451(12) 0.0199(9) -0.0084(9) -0.0049(8)
C41 0.0188(9) 0.0284(8) 0.0258(9) 0.0121(7) 0.0032(6) 0.0089(7)
C42 0.0161(9) 0.0253(8) 0.0227(8) 0.0080(7) -0.0009(6) 0.0060(7)
C43 0.0212(9) 0.0241(8) 0.0201(8) 0.0095(6) -0.0006(6) 0.0090(7)
C44 0.0280(10) 0.0209(8) 0.0221(8) 0.0074(6) -0.0028(7) 0.0087(7)
C45 0.0267(10) 0.0286(8) 0.0188(8) 0.0081(7) 0.0015(7) 0.0120(7)
C46 0.0247(11) 0.0443(11) 0.0463(12) 0.0255(10) 0.0132(9) 0.0108(9)
C47 0.0290(12) 0.0327(10) 0.0269(10) 0.0031(8) -0.0064(8) 0.0021(9)
C48 0.0315(12) 0.0377(10) 0.0286(10) 0.0201(8) 0.0029(8) 0.0114(9)
C49 0.0514(15) 0.0208(9) 0.0343(11) 0.0084(8) -0.0108(9) 0.0029(9)
C50 0.0463(14) 0.0463(12) 0.0212(10) 0.0087(9) 0.0052(8) 0.0211(11)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Ti1 C2 2.2828(17) . ?
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Ti1 C3 2.4181(19) . ?
Ti1 C4 2.428(2) . ?
Ti1 C6 2.5475(15) . ?
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C1 C5 1.440(3) . ?
C1 C2 1.458(2) . ?
C2 C3 1.403(3) . ?
C3 C4 1.402(3) . ?
C4 C5 1.412(3) . ?
C6 C11 1.523(2) . ?
C6 C7 1.533(2) . ?
C7 C8 1.531(3) . ?
C7 C14 1.552(2) . ?
C8 C9 1.533(3) . ?
C9 C10 1.534(2) . ?
C9 C15 1.539(3) . ?
C10 C11 1.533(3) . ?
C11 C12 1.551(2) . ?
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C12 C13 1.537(3) . ?
C13 C15 1.532(3) . ?
C13 C14 1.535(3) . ?
C16 C20 1.410(2) . ?
C16 C17 1.422(2) . ?
C16 C21 1.503(2) . ?
C17 C18 1.418(2) . ?
C17 C22 1.506(3) . ?
C18 C19 1.420(2) . ?
C18 C23 1.508(2) . ?
C19 C20 1.425(2) . ?
C19 C24 1.504(2) . ?
C20 C25 1.501(3) . ?
Ti2 C26 2.1797(14) . ?
Ti2 C27 2.2871(17) . ?
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C18 Ti1 C5 C1 77.97(13) . . . . ?
C3 Ti1 C5 C1 82.28(12) . . . . ?
C4 Ti1 C5 C1 117.42(18) . . . . ?
C6 Ti1 C5 C1 -31.62(10) . . . . ?
C5 C1 C6 C11 171.54(14) . . . . ?
C2 C1 C6 C11 -47.5(2) . . . . ?
Ti1 C1 C6 C11 -116.88(13) . . . . ?
C5 C1 C6 C7 32.4(2) . . . . ?
C2 C1 C6 C7 173.35(15) . . . . ?
Ti1 C1 C6 C7 103.95(13) . . . . ?
C5 C1 C6 Ti1 -71.58(14) . . . . ?
C2 C1 C6 Ti1 69.40(14) . . . . ?
C2 Ti1 C6 C1 -34.28(11) . . . . ?
C5 Ti1 C6 C1 34.41(11) . . . . ?
Cl1 Ti1 C6 C1 107.54(10) . . . . ?
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C17 Ti1 C6 C1 -123.03(14) . . . . ?
C20 Ti1 C6 C1 -153.56(11) . . . . ?
C16 Ti1 C6 C1 -169.10(10) . . . . ?
C19 Ti1 C6 C1 -119.07(11) . . . . ?
C18 Ti1 C6 C1 -96.60(11) . . . . ?
C3 Ti1 C6 C1 -16.22(12) . . . . ?
C4 Ti1 C6 C1 17.44(12) . . . . ?
C1 Ti1 C6 C11 105.55(18) . . . . ?
C2 Ti1 C6 C11 71.27(14) . . . . ?
C5 Ti1 C6 C11 139.96(16) . . . . ?
Cl1 Ti1 C6 C11 -146.92(13) . . . . ?
C17 Ti1 C6 C11 -17.5(2) . . . . ?
C20 Ti1 C6 C11 -48.01(14) . . . . ?
C16 Ti1 C6 C11 -63.56(16) . . . . ?
C19 Ti1 C6 C11 -13.53(14) . . . . ?
C18 Ti1 C6 C11 8.95(16) . . . . ?
C3 Ti1 C6 C11 89.32(15) . . . . ?
C4 Ti1 C6 C11 122.99(15) . . . . ?
C1 Ti1 C6 C7 -109.63(16) . . . . ?
C2 Ti1 C6 C7 -143.91(14) . . . . ?
C5 Ti1 C6 C7 -75.22(13) . . . . ?
Cl1 Ti1 C6 C7 -2.09(12) . . . . ?
C17 Ti1 C6 C7 127.34(14) . . . . ?
C20 Ti1 C6 C7 96.82(12) . . . . ?
C16 Ti1 C6 C7 81.27(13) . . . . ?
C19 Ti1 C6 C7 131.30(12) . . . . ?
C18 Ti1 C6 C7 153.77(11) . . . . ?
C3 Ti1 C6 C7 -125.85(13) . . . . ?
C4 Ti1 C6 C7 -92.19(13) . . . . ?
C1 C6 C7 C8 -161.58(15) . . . . ?
C11 C6 C7 C8 55.79(18) . . . . ?
Ti1 C6 C7 C8 -94.53(15) . . . . ?
C1 C6 C7 C14 79.54(19) . . . . ?
C11 C6 C7 C14 -63.09(18) . . . . ?
Ti1 C6 C7 C14 146.59(12) . . . . ?
C6 C7 C8 C9 -58.87(18) . . . . ?
C14 C7 C8 C9 59.53(18) . . . . ?
C7 C8 C9 C10 60.17(18) . . . . ?
C7 C8 C9 C15 -59.81(18) . . . . ?
C8 C9 C10 C11 -59.49(19) . . . . ?
C15 C9 C10 C11 60.5(2) . . . . ?
C1 C6 C11 C10 161.95(14) . . . . ?
C7 C6 C11 C10 -55.66(17) . . . . ?
Ti1 C6 C11 C10 90.70(15) . . . . ?
C1 C6 C11 C12 -79.51(17) . . . . ?
C7 C6 C11 C12 62.89(17) . . . . ?
Ti1 C6 C11 C12 -150.75(12) . . . . ?
C9 C10 C11 C6 58.23(18) . . . . ?
C9 C10 C11 C12 -59.94(19) . . . . ?
C6 C11 C12 C13 -60.54(19) . . . . ?
C10 C11 C12 C13 60.16(19) . . . . ?
C11 C12 C13 C15 -60.6(2) . . . . ?
C11 C12 C13 C14 59.4(2) . . . . ?
C15 C13 C14 C7 60.75(19) . . . . ?
C12 C13 C14 C7 -59.1(2) . . . . ?
C8 C7 C14 C13 -59.95(19) . . . . ?
C6 C7 C14 C13 60.3(2) . . . . ?
C14 C13 C15 C9 -60.26(19) . . . . ?
C12 C13 C15 C9 59.7(2) . . . . ?
C8 C9 C15 C13 59.6(2) . . . . ?
C10 C9 C15 C13 -59.8(2) . . . . ?
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C1 Ti1 C16 C20 5.9(3) . . . . ?
C2 Ti1 C16 C20 -68.58(14) . . . . ?
C5 Ti1 C16 C20 145.49(16) . . . . ?
Cl1 Ti1 C16 C20 120.08(9) . . . . ?
C17 Ti1 C16 C20 -116.98(13) . . . . ?
C19 Ti1 C16 C20 -37.67(9) . . . . ?
C18 Ti1 C16 C20 -78.87(10) . . . . ?
C3 Ti1 C16 C20 -115.80(11) . . . . ?
C4 Ti1 C16 C20 -161.27(11) . . . . ?
C6 Ti1 C16 C20 28.14(12) . . . . ?
C1 Ti1 C16 C17 122.8(2) . . . . ?
C2 Ti1 C16 C17 48.39(15) . . . . ?
C5 Ti1 C16 C17 -97.53(18) . . . . ?
Cl1 Ti1 C16 C17 -122.94(10) . . . . ?
C20 Ti1 C16 C17 116.98(13) . . . . ?
C19 Ti1 C16 C17 79.30(10) . . . . ?
C18 Ti1 C16 C17 38.11(10) . . . . ?
C3 Ti1 C16 C17 1.18(14) . . . . ?
C4 Ti1 C16 C17 -44.29(14) . . . . ?
C6 Ti1 C16 C17 145.11(10) . . . . ?
C1 Ti1 C16 C21 -115.3(2) . . . . ?
C2 Ti1 C16 C21 170.23(16) . . . . ?
C5 Ti1 C16 C21 24.3(3) . . . . ?
Cl1 Ti1 C16 C21 -1.11(17) . . . . ?
C17 Ti1 C16 C21 121.8(2) . . . . ?
C20 Ti1 C16 C21 -121.2(2) . . . . ?
C19 Ti1 C16 C21 -158.86(19) . . . . ?
C18 Ti1 C16 C21 159.9(2) . . . . ?
C3 Ti1 C16 C21 123.01(18) . . . . ?
C4 Ti1 C16 C21 77.5(2) . . . . ?
C6 Ti1 C16 C21 -93.05(18) . . . . ?
C20 C16 C17 C18 -3.01(17) . . . . ?
C21 C16 C17 C18 169.40(16) . . . . ?
Ti1 C16 C17 C18 -67.06(11) . . . . ?
C20 C16 C17 C22 -178.41(16) . . . . ?
C21 C16 C17 C22 -6.0(3) . . . . ?
Ti1 C16 C17 C22 117.54(17) . . . . ?
C20 C16 C17 Ti1 64.05(11) . . . . ?
C21 C16 C17 Ti1 -123.54(17) . . . . ?
C1 Ti1 C17 C18 -36.68(19) . . . . ?
C2 Ti1 C17 C18 -34.73(13) . . . . ?
C5 Ti1 C17 C18 -105.45(14) . . . . ?
Cl1 Ti1 C17 C18 170.68(10) . . . . ?
C20 Ti1 C17 C18 77.75(11) . . . . ?
C16 Ti1 C17 C18 114.04(15) . . . . ?
C19 Ti1 C17 C18 36.66(10) . . . . ?
C3 Ti1 C17 C18 -65.04(12) . . . . ?
C4 Ti1 C17 C18 -96.72(12) . . . . ?
C6 Ti1 C17 C18 41.34(18) . . . . ?
C1 Ti1 C17 C16 -150.72(13) . . . . ?
C2 Ti1 C17 C16 -148.77(10) . . . . ?
C5 Ti1 C17 C16 140.50(12) . . . . ?
Cl1 Ti1 C17 C16 56.63(10) . . . . ?
C20 Ti1 C17 C16 -36.30(9) . . . . ?
C19 Ti1 C17 C16 -77.39(10) . . . . ?
C18 Ti1 C17 C16 -114.04(15) . . . . ?
C3 Ti1 C17 C16 -179.08(11) . . . . ?
C4 Ti1 C17 C16 149.23(11) . . . . ?
C6 Ti1 C17 C16 -72.70(16) . . . . ?
C1 Ti1 C17 C22 87.5(2) . . . . ?
C2 Ti1 C17 C22 89.42(16) . . . . ?
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C5 Ti1 C17 C22 18.7(2) . . . . ?
Cl1 Ti1 C17 C22 -65.17(15) . . . . ?
C20 Ti1 C17 C22 -158.11(17) . . . . ?
C16 Ti1 C17 C22 -121.81(19) . . . . ?
C19 Ti1 C17 C22 160.80(18) . . . . ?
C18 Ti1 C17 C22 124.1(2) . . . . ?
C3 Ti1 C17 C22 59.11(16) . . . . ?
C4 Ti1 C17 C22 27.42(17) . . . . ?
C6 Ti1 C17 C22 165.49(14) . . . . ?
C16 C17 C18 C19 2.78(17) . . . . ?
C22 C17 C18 C19 178.07(16) . . . . ?
Ti1 C17 C18 C19 -64.10(11) . . . . ?
C16 C17 C18 C23 -168.25(17) . . . . ?
C22 C17 C18 C23 7.0(3) . . . . ?
Ti1 C17 C18 C23 124.87(18) . . . . ?
C16 C17 C18 Ti1 66.89(10) . . . . ?
C22 C17 C18 Ti1 -117.83(18) . . . . ?
C1 Ti1 C18 C17 160.56(10) . . . . ?
C2 Ti1 C18 C17 148.27(11) . . . . ?
C5 Ti1 C18 C17 117.28(12) . . . . ?
Cl1 Ti1 C18 C17 -12.56(13) . . . . ?
C20 Ti1 C18 C17 -79.22(11) . . . . ?
C16 Ti1 C18 C17 -38.29(10) . . . . ?
C19 Ti1 C18 C17 -116.63(14) . . . . ?
C3 Ti1 C18 C17 113.59(12) . . . . ?
C4 Ti1 C18 C17 94.96(11) . . . . ?
C6 Ti1 C18 C17 -159.21(10) . . . . ?
C1 Ti1 C18 C19 -82.81(11) . . . . ?
C2 Ti1 C18 C19 -95.10(10) . . . . ?
C5 Ti1 C18 C19 -126.09(11) . . . . ?
Cl1 Ti1 C18 C19 104.06(9) . . . . ?
C17 Ti1 C18 C19 116.63(14) . . . . ?
C20 Ti1 C18 C19 37.41(9) . . . . ?
C16 Ti1 C18 C19 78.34(10) . . . . ?
C3 Ti1 C18 C19 -129.78(10) . . . . ?
C4 Ti1 C18 C19 -148.41(10) . . . . ?
C6 Ti1 C18 C19 -42.58(11) . . . . ?
C1 Ti1 C18 C23 39.1(2) . . . . ?
C2 Ti1 C18 C23 26.79(18) . . . . ?
C5 Ti1 C18 C23 -4.2(2) . . . . ?
Cl1 Ti1 C18 C23 -134.05(16) . . . . ?
C17 Ti1 C18 C23 -121.5(2) . . . . ?
C20 Ti1 C18 C23 159.3(2) . . . . ?
C16 Ti1 C18 C23 -159.8(2) . . . . ?
C19 Ti1 C18 C23 121.9(2) . . . . ?
C3 Ti1 C18 C23 -7.89(18) . . . . ?
C4 Ti1 C18 C23 -26.53(19) . . . . ?
C6 Ti1 C18 C23 79.30(19) . . . . ?
C17 C18 C19 C20 -1.53(17) . . . . ?
C23 C18 C19 C20 169.56(16) . . . . ?
Ti1 C18 C19 C20 -64.73(10) . . . . ?
C17 C18 C19 C24 -171.00(16) . . . . ?
C23 C18 C19 C24 0.1(3) . . . . ?
Ti1 C18 C19 C24 125.80(16) . . . . ?
C17 C18 C19 Ti1 63.20(11) . . . . ?
C23 C18 C19 Ti1 -125.71(17) . . . . ?
C1 Ti1 C19 C18 113.59(10) . . . . ?
C2 Ti1 C19 C18 82.58(10) . . . . ?
C5 Ti1 C19 C18 99.40(14) . . . . ?
Cl1 Ti1 C19 C18 -108.04(9) . . . . ?
C17 Ti1 C19 C18 -36.86(9) . . . . ?
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C20 Ti1 C19 C18 -115.61(13) . . . . ?
C16 Ti1 C19 C18 -78.32(10) . . . . ?
C3 Ti1 C19 C18 50.88(10) . . . . ?
C4 Ti1 C19 C18 45.39(13) . . . . ?
C6 Ti1 C19 C18 145.26(9) . . . . ?
C1 Ti1 C19 C20 -130.80(10) . . . . ?
C2 Ti1 C19 C20 -161.82(10) . . . . ?
C5 Ti1 C19 C20 -145.00(12) . . . . ?
Cl1 Ti1 C19 C20 7.56(11) . . . . ?
C17 Ti1 C19 C20 78.74(10) . . . . ?
C16 Ti1 C19 C20 37.29(9) . . . . ?
C18 Ti1 C19 C20 115.61(13) . . . . ?
C3 Ti1 C19 C20 166.49(10) . . . . ?
C4 Ti1 C19 C20 160.99(10) . . . . ?
C6 Ti1 C19 C20 -99.14(9) . . . . ?
C1 Ti1 C19 C24 -6.88(18) . . . . ?
C2 Ti1 C19 C24 -37.90(17) . . . . ?
C5 Ti1 C19 C24 -21.1(2) . . . . ?
Cl1 Ti1 C19 C24 131.48(15) . . . . ?
C17 Ti1 C19 C24 -157.34(19) . . . . ?
C20 Ti1 C19 C24 123.9(2) . . . . ?
C16 Ti1 C19 C24 161.20(19) . . . . ?
C18 Ti1 C19 C24 -120.5(2) . . . . ?
C3 Ti1 C19 C24 -69.60(17) . . . . ?
C4 Ti1 C19 C24 -75.09(18) . . . . ?
C6 Ti1 C19 C24 24.78(17) . . . . ?
C17 C16 C20 C19 2.07(17) . . . . ?
C21 C16 C20 C19 -170.45(15) . . . . ?
Ti1 C16 C20 C19 65.25(10) . . . . ?
C17 C16 C20 C25 175.05(15) . . . . ?
C21 C16 C20 C25 2.5(2) . . . . ?
Ti1 C16 C20 C25 -121.77(15) . . . . ?
C17 C16 C20 Ti1 -63.18(11) . . . . ?
C21 C16 C20 Ti1 124.30(16) . . . . ?
C18 C19 C20 C16 -0.34(17) . . . . ?
C24 C19 C20 C16 168.75(16) . . . . ?
Ti1 C19 C20 C16 -65.25(11) . . . . ?
C18 C19 C20 C25 -172.91(15) . . . . ?
C24 C19 C20 C25 -3.8(3) . . . . ?
Ti1 C19 C20 C25 122.17(16) . . . . ?
C18 C19 C20 Ti1 64.92(11) . . . . ?
C24 C19 C20 Ti1 -125.99(16) . . . . ?
C1 Ti1 C20 C16 -177.87(9) . . . . ?
C2 Ti1 C20 C16 136.47(9) . . . . ?
C5 Ti1 C20 C16 -137.2(2) . . . . ?
Cl1 Ti1 C20 C16 -59.06(9) . . . . ?
C17 Ti1 C20 C16 36.85(9) . . . . ?
C19 Ti1 C20 C16 115.23(13) . . . . ?
C18 Ti1 C20 C16 78.03(10) . . . . ?
C3 Ti1 C20 C16 96.22(12) . . . . ?
C4 Ti1 C20 C16 56.9(3) . . . . ?
C6 Ti1 C20 C16 -158.90(9) . . . . ?
C1 Ti1 C20 C19 66.90(12) . . . . ?
C2 Ti1 C20 C19 21.24(11) . . . . ?
C5 Ti1 C20 C19 107.6(2) . . . . ?
Cl1 Ti1 C20 C19 -174.29(9) . . . . ?
C17 Ti1 C20 C19 -78.38(10) . . . . ?
C16 Ti1 C20 C19 -115.23(13) . . . . ?
C18 Ti1 C20 C19 -37.20(9) . . . . ?
C3 Ti1 C20 C19 -19.01(14) . . . . ?
C4 Ti1 C20 C19 -58.3(3) . . . . ?
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C6 Ti1 C20 C19 85.87(10) . . . . ?
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C2 Ti1 C20 C25 -103.85(16) . . . . ?
C5 Ti1 C20 C25 -17.5(3) . . . . ?
Cl1 Ti1 C20 C25 60.62(15) . . . . ?
C17 Ti1 C20 C25 156.52(17) . . . . ?
C16 Ti1 C20 C25 119.68(19) . . . . ?
C19 Ti1 C20 C25 -125.09(19) . . . . ?
C18 Ti1 C20 C25 -162.30(18) . . . . ?
C3 Ti1 C20 C25 -144.11(15) . . . . ?
C4 Ti1 C20 C25 176.6(2) . . . . ?
C6 Ti1 C20 C25 -39.23(16) . . . . ?
C27 Ti2 C26 C30 109.99(15) . . . . ?
C44 Ti2 C26 C30 103.18(13) . . . . ?
Cl2 Ti2 C26 C30 -52.64(10) . . . . ?
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C29 Ti2 C26 C30 35.29(11) . . . . ?
C28 Ti2 C26 C30 73.93(11) . . . . ?
C41 Ti2 C26 C30 172.05(9) . . . . ?
C42 Ti2 C26 C30 -157.28(10) . . . . ?
C31 Ti2 C26 C30 -124.64(14) . . . . ?
C27 Ti2 C26 C31 -125.37(16) . . . . ?
C30 Ti2 C26 C31 124.64(14) . . . . ?
C44 Ti2 C26 C31 -132.18(11) . . . . ?
Cl2 Ti2 C26 C31 71.99(10) . . . . ?
C45 Ti2 C26 C31 -101.52(10) . . . . ?
C43 Ti2 C26 C31 -62.7(4) . . . . ?
C29 Ti2 C26 C31 159.93(12) . . . . ?
C28 Ti2 C26 C31 -161.44(13) . . . . ?
C41 Ti2 C26 C31 -63.31(11) . . . . ?
C42 Ti2 C26 C31 -32.64(14) . . . . ?
C30 Ti2 C26 C27 -109.99(15) . . . . ?
C44 Ti2 C26 C27 -6.81(17) . . . . ?
Cl2 Ti2 C26 C27 -162.63(10) . . . . ?
C45 Ti2 C26 C27 23.85(13) . . . . ?
C43 Ti2 C26 C27 62.7(4) . . . . ?
C29 Ti2 C26 C27 -74.70(12) . . . . ?
C28 Ti2 C26 C27 -36.06(11) . . . . ?
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C42 Ti2 C26 C27 92.73(13) . . . . ?
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C30 C26 C27 C28 -2.61(17) . . . . ?
C31 C26 C27 C28 142.04(15) . . . . ?
Ti2 C26 C27 C28 68.59(12) . . . . ?
C30 C26 C27 Ti2 -71.20(10) . . . . ?
C31 C26 C27 Ti2 73.45(13) . . . . ?
C26 Ti2 C27 C28 -115.80(17) . . . . ?
C30 Ti2 C27 C28 -74.87(12) . . . . ?
C44 Ti2 C27 C28 59.97(13) . . . . ?
Cl2 Ti2 C27 C28 -89.24(12) . . . . ?
C45 Ti2 C27 C28 85.59(12) . . . . ?
C43 Ti2 C27 C28 75.14(15) . . . . ?
C29 Ti2 C27 C28 -34.42(11) . . . . ?
C41 Ti2 C27 C28 117.35(12) . . . . ?
C42 Ti2 C27 C28 120.24(12) . . . . ?
C31 Ti2 C27 C28 -147.26(13) . . . . ?
C30 Ti2 C27 C26 40.93(10) . . . . ?
C44 Ti2 C27 C26 175.77(10) . . . . ?
Cl2 Ti2 C27 C26 26.56(15) . . . . ?
C45 Ti2 C27 C26 -158.62(12) . . . . ?
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C43 Ti2 C27 C26 -169.07(10) . . . . ?
C29 Ti2 C27 C26 81.38(11) . . . . ?
C28 Ti2 C27 C26 115.80(17) . . . . ?
C41 Ti2 C27 C26 -126.85(11) . . . . ?
C42 Ti2 C27 C26 -123.97(11) . . . . ?
C31 Ti2 C27 C26 -31.46(10) . . . . ?
C26 C27 C28 C29 0.61(19) . . . . ?
Ti2 C27 C28 C29 61.56(13) . . . . ?
C26 C27 C28 Ti2 -60.95(11) . . . . ?
C26 Ti2 C28 C29 -79.96(11) . . . . ?
C27 Ti2 C28 C29 -119.59(16) . . . . ?
C30 Ti2 C28 C29 -36.40(11) . . . . ?
C44 Ti2 C28 C29 117.10(11) . . . . ?
Cl2 Ti2 C28 C29 4.59(13) . . . . ?
C45 Ti2 C28 C29 151.52(12) . . . . ?
C43 Ti2 C28 C29 109.54(11) . . . . ?
C41 Ti2 C28 C29 170.98(10) . . . . ?
C42 Ti2 C28 C29 148.52(11) . . . . ?
C31 Ti2 C28 C29 -90.51(11) . . . . ?
C26 Ti2 C28 C27 39.63(11) . . . . ?
C30 Ti2 C28 C27 83.18(12) . . . . ?
C44 Ti2 C28 C27 -123.32(12) . . . . ?
Cl2 Ti2 C28 C27 124.17(11) . . . . ?
C45 Ti2 C28 C27 -88.89(12) . . . . ?
C43 Ti2 C28 C27 -130.87(11) . . . . ?
C29 Ti2 C28 C27 119.59(16) . . . . ?
C41 Ti2 C28 C27 -69.43(12) . . . . ?
C42 Ti2 C28 C27 -91.90(13) . . . . ?
C31 Ti2 C28 C27 29.08(12) . . . . ?
C27 C28 C29 C30 1.7(2) . . . . ?
Ti2 C28 C29 C30 59.23(12) . . . . ?
C27 C28 C29 Ti2 -57.52(12) . . . . ?
C26 Ti2 C29 C28 80.17(12) . . . . ?
C27 Ti2 C29 C28 35.68(11) . . . . ?
C30 Ti2 C29 C28 118.16(17) . . . . ?
C44 Ti2 C29 C28 -65.26(11) . . . . ?
Cl2 Ti2 C29 C28 -176.40(10) . . . . ?
C45 Ti2 C29 C28 -30.03(12) . . . . ?
C43 Ti2 C29 C28 -92.94(12) . . . . ?
C41 Ti2 C29 C28 -13.83(16) . . . . ?
C42 Ti2 C29 C28 -76.9(2) . . . . ?
C31 Ti2 C29 C28 91.55(11) . . . . ?
C26 Ti2 C29 C30 -37.99(12) . . . . ?
C27 Ti2 C29 C30 -82.48(13) . . . . ?
C44 Ti2 C29 C30 176.58(12) . . . . ?
Cl2 Ti2 C29 C30 65.44(12) . . . . ?
C45 Ti2 C29 C30 -148.19(12) . . . . ?
C43 Ti2 C29 C30 148.89(11) . . . . ?
C28 Ti2 C29 C30 -118.16(17) . . . . ?
C41 Ti2 C29 C30 -131.99(12) . . . . ?
C42 Ti2 C29 C30 164.96(16) . . . . ?
C31 Ti2 C29 C30 -26.61(13) . . . . ?
C28 C29 C30 C26 -3.4(2) . . . . ?
Ti2 C29 C30 C26 59.35(11) . . . . ?
C28 C29 C30 Ti2 -62.77(13) . . . . ?
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  University of Groningen,
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 Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
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  NL-9747 AG Groningen, The Netherlands.
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Refinement was frustrated by a disorder problem: from the solution it was clear
that the toluene solvent molecule was highly disordered over an inversion
center. The electron density appeared to be spread out, indicating
transformational disorder. No satisfactory discrete model could be fitted in
this density. The BYPASS procedure was used to take into account the
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count of 94 within a volume of 335.9 \%A^3^ in the unit cell.
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Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S. Gould, R.O.
Isra\"el, R. & Smits, J.M.M.  (1999). The <i>DIRDIF99</i> program system,
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Meetsma, A. (2003). Extended version of the program <i>PLUTO</i>. Groningen
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University of G\"ottingen, Germany, 1997.

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Fig. 1. Perspective <i>PLUTO</i> drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective <i>ORTEP</i> drawing of the title compound. Displacement
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have been omitted to improve clarity.
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'C25 H34 Ti, C24 H20 B'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural          ?
_chemical_formula_sum
'C49 H54 B Ti'
_chemical_formula_iupac               ?
_chemical_formula_weight                 701.66
_chemical_compound_source            'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Ti  Ti    0.2776    0.4457
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 B   B    0.0013    0.0007
 '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 2ybc'
_symmetry_space_group_name_H-M       'P 21/c'
_symmetry_Int_Tables_number                14

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

_cell_length_a                        11.0183(5)
_cell_length_b                        19.4775(9)
_cell_length_c                        18.3684(8)
_cell_angle_alpha                     90
_cell_angle_beta                      95.452(1)
_cell_angle_gamma                     90
_cell_volume                         3924.2(3)
_cell_formula_units_Z                 4

_cell_measurement_temperature    100(1)
```

```
_cell_measurement_reflns_used      6844
_cell_measurement_theta_min        2.32
_cell_measurement_theta_max       26.30
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   6844 reflections after integration using the SAINT software
   package (Bruker, 2001).
;

_exptl_crystal_description       'platelet'
_exptl_crystal_colour            'green'
_exptl_crystal_size_max           0.25
_exptl_crystal_size_mid           0.25
_exptl_crystal_size_min           0.055
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.188
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1500
_exptl_absorpt_coefficient_mu     0.251
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    'SADABS, (Bruker, 2001))'
_exptl_absorpt_correction_T_min   0.9341
_exptl_absorpt_correction_T_max   0.9863


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

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method            'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2001)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?

loop_
_diffrn_standard_refln_index_h
```

```
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number             37685
_diffrn_reflns_av_R_equivalents   0.0471
_diffrn_reflns_av_sigmaI/netI     0.0582
_diffrn_reflns_limit_h_min        -14
_diffrn_reflns_limit_h_max        14
_diffrn_reflns_limit_k_min        -25
_diffrn_reflns_limit_k_max        25
_diffrn_reflns_limit_l_min        -25
_diffrn_reflns_limit_l_max        24
_diffrn_reflns_theta_min          2.32
_diffrn_reflns_theta_max          28.28
_diffrn_measured_fraction_theta_max    0.988
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.992

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

# number of unique reflections
_reflns_number_total              9627
_reflns_number_gt                 7339
_reflns_threshold_expression      I>2\s(I)


_computing_data_collection          'SMART, (Bruker, 2001)'
_computing_cell_refinement          'SAINT-Plus, (Bruker, 2001)'
_computing_data_reduction           'SAINT-Plus'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 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            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0756P)^2^+0.4366P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    difmap
_refine_ls_hydrogen_treatment     refall
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?

_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          9627
_refine_ls_number_parameters      676
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0670
_refine_ls_R_factor_gt            0.0492
_refine_ls_wR_factor_ref          0.1323
_refine_ls_wR_factor_gt           0.1250
_refine_ls_goodness_of_fit_ref    1.033
_refine_ls_restrained_S_all       1.033
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.436
_refine_diff_density_min         -0.256
_refine_diff_density_rms          0.068


_vrn_publ_code_squeezed_elec       94
_vrn_publ_code_void_volume        335.9
_vrn_publ_code_frame_time_sec      10.0
_vrn_publ_code_meas_time_hour       8.0

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

# 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
Ti1 Ti Uani 0.17010(3) 0.19187(1) 0.35004(2) 1.000 0.0155(1) . .
C11 C Uani 0.26206(15) 0.08587(8) 0.32793(9) 1.000 0.0172(5) . .
C12 C Uani 0.16832(15) 0.07131(8) 0.37416(10) 1.000 0.0180(5) . .
C13 C Uani 0.19728(15) 0.10475(9) 0.44133(9) 1.000 0.0186(5) . .
C14 C Uani 0.31115(15) 0.13920(9) 0.43863(9) 1.000 0.0186(5) . .
```

```
C15 C Uani 0.34946(15) 0.12878(9) 0.36797(10) 1.000 0.0181(5) . .
C16 C Uani 0.27747(17) 0.05248(9) 0.25612(10) 1.000 0.0214(5) . .
C17 C Uani 0.06541(17) 0.02140(10) 0.35955(11) 1.000 0.0234(5) . .
C18 C Uani 0.12563(18) 0.09646(11) 0.50636(10) 1.000 0.0242(5) . .
C19 C Uani 0.38415(18) 0.17131(11) 0.50230(11) 1.000 0.0252(5) . .
C110 C Uani 0.46622(17) 0.15447(11) 0.34150(12) 1.000 0.0249(6) . .
C111 C Uani 0.06783(16) 0.29620(9) 0.33398(10) 1.000 0.0184(5) . .
C112 C Uani 0.02855(17) 0.26315(9) 0.39631(10) 1.000 0.0218(5) . .
C113 C Uani 0.12885(17) 0.25900(9) 0.44905(10) 1.000 0.0228(5) . .
C114 C Uani 0.23058(17) 0.28957(9) 0.41997(10) 1.000 0.0204(5) . .
C115 C Uani 0.19341(15) 0.31389(8) 0.34896(9) 1.000 0.0172(5) . .
C116 C Uani 0.27218(15) 0.35089(9) 0.29803(10) 1.000 0.0189(5) . .
C117 C Uani 0.38626(16) 0.38494(9) 0.33796(11) 1.000 0.0232(5) . .
C118 C Uani 0.35040(18) 0.44425(10) 0.38640(11) 1.000 0.0258(6) . .
C119 C Uani 0.27891(17) 0.49854(9) 0.33946(10) 1.000 0.0238(5) . .
C120 C Uani 0.35837(18) 0.52645(9) 0.28160(11) 1.000 0.0240(5) . .
C121 C Uani 0.39434(17) 0.46753(9) 0.23320(10) 1.000 0.0235(5) . .
C122 C Uani 0.46565(17) 0.41341(10) 0.28056(12) 1.000 0.0274(6) . .
C123 C Uani 0.28013(18) 0.43448(10) 0.19495(10) 1.000 0.0243(5) . .
C124 C Uani 0.19972(16) 0.40625(9) 0.25177(10) 1.000 0.0201(5) . .
C125 C Uani 0.16444(16) 0.46479(9) 0.30123(11) 1.000 0.0228(5) . .
C21 C Uani 0.74433(14) 0.31010(8) 0.24100(9) 1.000 0.0164(4) . .
C22 C Uani 0.79997(15) 0.37240(9) 0.26329(10) 1.000 0.0180(5) . .
C23 C Uani 0.80579(16) 0.39537(10) 0.33508(10) 1.000 0.0219(5) . .
C24 C Uani 0.75444(16) 0.35692(10) 0.38738(10) 1.000 0.0230(5) . .
C25 C Uani 0.69914(16) 0.29515(10) 0.36766(10) 1.000 0.0222(5) . .
C26 C Uani 0.69533(15) 0.27222(9) 0.29596(10) 1.000 0.0191(5) . .
C27 C Uani 0.64874(14) 0.22448(8) 0.13070(9) 1.000 0.0155(4) . .
C28 C Uani 0.52810(15) 0.22935(9) 0.14896(10) 1.000 0.0188(5) . .
C29 C Uani 0.43639(16) 0.18567(9) 0.11944(10) 1.000 0.0219(5) . .
C210 C Uani 0.46134(16) 0.13550(9) 0.06964(10) 1.000 0.0223(5) . .
C211 C Uani 0.57904(16) 0.12975(9) 0.04968(10) 1.000 0.0217(5) . .
C212 C Uani 0.66993(16) 0.17310(9) 0.08042(10) 1.000 0.0198(5) . .
C213 C Uani 0.89037(15) 0.24576(8) 0.16771(9) 1.000 0.0153(4) . .
C214 C Uani 0.90985(15) 0.18546(8) 0.20897(9) 1.000 0.0168(5) . .
C215 C Uani 1.02506(16) 0.15871(9) 0.22850(9) 1.000 0.0187(5) . .
C216 C Uani 1.12838(16) 0.19292(9) 0.20776(10) 1.000 0.0189(5) . .
C217 C Uani 1.11243(15) 0.25204(9) 0.16570(10) 1.000 0.0190(5) . .
C218 C Uani 0.99628(15) 0.27726(9) 0.14598(9) 1.000 0.0161(5) . .
C219 C Uani 0.73817(14) 0.34092(8) 0.09522(9) 1.000 0.0165(4) . .
C220 C Uani 0.78169(16) 0.33288(10) 0.02626(10) 1.000 0.0214(5) . .
C221 C Uani 0.75726(18) 0.38036(11) -0.02957(11) 1.000 0.0278(6) . .
C222 C Uani 0.68918(18) 0.43865(10) -0.01891(11) 1.000 0.0288(6) . .
C223 C Uani 0.64397(18) 0.44815(9) 0.04829(11) 1.000 0.0263(5) . .
C224 C Uani 0.66822(16) 0.40030(9) 0.10361(10) 1.000 0.0209(5) . .
B2 B Uani 0.75389(16) 0.28063(9) 0.15788(10) 1.000 0.0150(5) . .

H110' H Uiso 0.46384 0.15792 0.28916 1.00(4) 0.042(2) . .
H110" H Uiso 0.53263 0.12467 0.35564 1.00(5) 0.067(3) . .
H118' H Uiso 0.30256 0.42514 0.42357 1.00(4) 0.0285(19) . .
H120' H Uiso 0.43138 0.54948 0.30594 1.00(4) 0.033(2) . .
H122' H Uiso 0.49595 0.37717 0.24860 1.00(3) 0.0175(17) . .
H123' H Uiso 0.23072 0.46946 0.16313 1.00(4) 0.0236(18) . .
H125' H Uiso 0.11811 0.50049 0.27217 1.00(4) 0.0209(18) . .
H16 H Uiso 0.33196 0.07906 0.22771 1.00(4) 0.0267(19) . .
H16' H Uiso 0.20327 0.04844 0.22704 1.00(4) 0.036(2) . .
H16" H Uiso 0.30917 0.00284 0.26602 1.00(4) 0.039(2) . .
H17 H Uiso 0.08304 -0.02039 0.39190 1.00(4) 0.039(2) . .
H17' H Uiso 0.05121 0.00534 0.30469 1.00(4) 0.0352(19) . .
H17" H Uiso -0.00985 0.04137 0.37403 1.00(4) 0.038(2) . .
H18 H Uiso 0.03852 0.10697 0.49694 1.00(4) 0.028(2) . .
```

```
H18' H Uiso 0.15851 0.12991 0.54712 1.00(4) 0.037(2) . .
H18" H Uiso 0.13742 0.04976 0.52007 1.00(5) 0.059(2) . .
H19 H Uiso 0.42560 0.13782 0.52847 1.00(5) 0.050(2) . .
H19' H Uiso 0.33072 0.19613 0.53724 1.00(5) 0.048(2) . .
H19" H Uiso 0.44524 0.20220 0.48387 1.00(4) 0.039(2) . .
H110 H Uiso 0.48423 0.20361 0.35724 1.00(5) 0.053(2) . .
H111 H Uiso 0.01912 0.30551 0.28793 1.00(4) 0.0218(19) . .
H112 H Uiso -0.05273 0.24707 0.40027 1.00(4) 0.0248(19) . .
H113 H Uiso 0.12705 0.23923 0.49858 1.00(4) 0.037(2) . .
H114 H Uiso 0.31008 0.29493 0.44560 1.00(4) 0.0184(18) . .
H116 H Uiso 0.29770 0.31606 0.26200 1.00(4) 0.0190(18) . .
H117 H Uiso 0.43516 0.35126 0.36799 1.00(3) 0.0189(17) . .
H118 H Uiso 0.43073 0.46489 0.41372 1.00(4) 0.0206(18) . .
H119 H Uiso 0.25591 0.53650 0.37070 1.00(4) 0.0229(18) . .
H120 H Uiso 0.31138 0.56034 0.24992 1.00(4) 0.039(2) . .
H121 H Uiso 0.44693 0.48361 0.19449 1.00(4) 0.0287(18) . .
H122 H Uiso 0.54305 0.43556 0.30764 1.00(4) 0.0295(19) . .
H123 H Uiso 0.30362 0.39793 0.16210 1.00(4) 0.0338(19) . .
H124 H Uiso 0.12832 0.38764 0.22703 1.00(4) 0.0181(18) . .
H125 H Uiso 0.11502 0.44648 0.34086 1.00(4) 0.0299(19) . .
H22 H Uiso 0.83525 0.39972 0.22766 1.00(3) 0.0202(17) . .
H23 H Uiso 0.84010 0.43756 0.34849 1.00(4) 0.0205(17) . .
H24 H Uiso 0.75716 0.37349 0.43902 1.00(4) 0.0253(18) . .
H25 H Uiso 0.66306 0.26590 0.40178 1.00(3) 0.0108(16) . .
H26 H Uiso 0.66540 0.23009 0.28540 1.00(4) 0.0206(18) . .
H28 H Uiso 0.50737 0.26196 0.18069 1.00(4) 0.0244(19) . .
H29 H Uiso 0.35580 0.19097 0.13269 1.00(4) 0.026(2) . .
H210 H Uiso 0.40005 0.10343 0.05192 1.00(4) 0.028(2) . .
H211 H Uiso 0.59727 0.09604 0.01861 1.00(4) 0.0263(19) . .
H212 H Uiso 0.75430 0.16718 0.06653 1.00(4) 0.0197(18) . .
H214 H Uiso 0.83829 0.15964 0.22755 1.00(3) 0.0159(17) . .
H215 H Uiso 1.03112 0.11264 0.25495 1.00(4) 0.0219(17) . .
H216 H Uiso 1.20551 0.17291 0.21844 1.00(4) 0.0233(19) . .
H217 H Uiso 1.18186 0.27406 0.15021 1.00(3) 0.0119(17) . .
H218 H Uiso 0.98800 0.31669 0.11790 1.00(3) 0.0088(16) . .
H220 H Uiso 0.83190 0.29062 0.01736 1.00(3) 0.0183(17) . .
H221 H Uiso 0.79053 0.37352 -0.07525 1.00(4) 0.0332(19) . .
H222 H Uiso 0.67207 0.47124 -0.05811 1.00(4) 0.0252(18) . .
H223 H Uiso 0.59265 0.48835 0.06031 1.00(4) 0.0231(18) . .
H224 H Uiso 0.63473 0.40876 0.14883 1.00(4) 0.0222(18) . .

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
Ti1 0.0142(2) 0.0156(2) 0.0161(2) 0.0005(1) -0.0016(1) 0.0008(1)
C11 0.0156(8) 0.0151(8) 0.0200(8) 0.0028(7) -0.0022(7) 0.0024(6)
C12 0.0155(8) 0.0160(8) 0.0219(8) 0.0040(7) -0.0009(7) 0.0019(6)
C13 0.0164(8) 0.0190(8) 0.0199(8) 0.0035(7) -0.0015(7) 0.0021(7)
C14 0.0151(8) 0.0194(8) 0.0203(9) 0.0024(7) -0.0036(7) 0.0028(6)
C15 0.0135(8) 0.0183(8) 0.0219(9) 0.0025(7) -0.0017(7) 0.0014(6)
C16 0.0216(9) 0.0192(9) 0.0230(9) -0.0011(7) 0.0003(8) 0.0029(7)
C17 0.0188(9) 0.0227(9) 0.0282(10) 0.0039(8) -0.0006(8) -0.0024(7)
C18 0.0239(9) 0.0284(10) 0.0204(9) 0.0068(8) 0.0022(8) 0.0037(8)
C19 0.0239(9) 0.0273(10) 0.0227(9) -0.0005(8) -0.0061(8) 0.0018(8)
C110 0.0167(9) 0.0300(10) 0.0281(10) 0.0020(8) 0.0021(8) -0.0012(8)
C111 0.0172(8) 0.0168(8) 0.0208(9) -0.0019(7) -0.0008(7) 0.0048(6)
```

```
C112 0.0194(9) 0.0220(9) 0.0242(9) -0.0023(7) 0.0033(7) 0.0017(7)
C113 0.0288(10) 0.0208(9) 0.0186(9) -0.0013(7) 0.0018(8) 0.0023(7)
C114 0.0223(9) 0.0188(8) 0.0191(8) -0.0022(7) -0.0032(7) 0.0010(7)
C115 0.0169(8) 0.0143(8) 0.0198(8) -0.0028(6) -0.0015(7) 0.0016(6)
C116 0.0199(8) 0.0166(8) 0.0199(9) -0.0022(7) -0.0002(7) 0.0001(7)
C117 0.0161(8) 0.0211(9) 0.0312(10) 0.0041(8) -0.0046(8) 0.0028(7)
C118 0.0281(10) 0.0263(10) 0.0212(9) 0.0001(8) -0.0067(8) -0.0056(8)
C119 0.0298(10) 0.0173(8) 0.0239(9) -0.0039(7) 0.0001(8) 0.0005(7)
C120 0.0253(9) 0.0192(9) 0.0262(10) 0.0018(8) -0.0041(8) -0.0030(7)
C121 0.0231(9) 0.0223(9) 0.0251(9) 0.0032(8) 0.0025(8) -0.0019(7)
C122 0.0180(9) 0.0248(10) 0.0395(11) 0.0044(9) 0.0036(8) 0.0012(7)
C123 0.0306(10) 0.0230(9) 0.0185(9) 0.0000(8) -0.0014(8) -0.0027(8)
C124 0.0199(8) 0.0198(8) 0.0193(9) 0.0003(7) -0.0043(7) -0.0030(7)
C125 0.0205(9) 0.0203(9) 0.0270(9) 0.0022(8) -0.0002(8) 0.0035(7)
C21 0.0125(7) 0.0187(8) 0.0174(8) 0.0015(7) -0.0011(6) 0.0030(6)
C22 0.0150(8) 0.0194(8) 0.0192(8) -0.0006(7) -0.0004(7) 0.0015(6)
C23 0.0203(8) 0.0208(9) 0.0237(9) -0.0039(7) -0.0026(7) 0.0021(7)
C24 0.0209(9) 0.0294(10) 0.0181(9) -0.0030(8) -0.0008(7) 0.0061(7)
C25 0.0194(8) 0.0284(9) 0.0187(8) 0.0038(8) 0.0016(7) 0.0030(7)
C26 0.0170(8) 0.0198(9) 0.0202(9) 0.0006(7) 0.0001(7) -0.0004(7)
C27 0.0145(7) 0.0157(8) 0.0157(8) 0.0045(6) -0.0021(6) 0.0005(6)
C28 0.0167(8) 0.0201(8) 0.0193(8) 0.0011(7) 0.0003(7) 0.0020(7)
C29 0.0147(8) 0.0277(9) 0.0228(9) 0.0066(7) -0.0009(7) -0.0007(7)
C210 0.0207(9) 0.0242(9) 0.0205(9) 0.0027(7) -0.0063(7) -0.0070(7)
C211 0.0237(9) 0.0205(9) 0.0205(9) -0.0047(7) -0.0003(7) -0.0033(7)
C212 0.0167(8) 0.0222(8) 0.0203(9) 0.0009(7) 0.0007(7) -0.0006(7)
C213 0.0155(8) 0.0172(8) 0.0130(7) -0.0033(6) 0.0004(6) -0.0005(6)
C214 0.0160(8) 0.0186(8) 0.0153(8) -0.0009(7) -0.0010(6) -0.0011(6)
C215 0.0212(8) 0.0170(8) 0.0176(8) 0.0005(7) 0.0005(7) 0.0016(7)
C216 0.0151(8) 0.0217(8) 0.0193(8) -0.0023(7) -0.0013(7) 0.0033(7)
C217 0.0157(8) 0.0219(9) 0.0195(8) -0.0018(7) 0.0021(7) -0.0034(7)
C218 0.0178(8) 0.0163(8) 0.0139(8) -0.0008(7) -0.0003(6) -0.0007(6)
C219 0.0131(7) 0.0170(8) 0.0183(8) 0.0001(7) -0.0046(6) -0.0034(6)
C220 0.0190(8) 0.0257(9) 0.0190(9) 0.0015(7) -0.0015(7) -0.0032(7)
C221 0.0255(9) 0.0377(11) 0.0192(9) 0.0067(8) -0.0032(8) -0.0091(8)
C222 0.0297(10) 0.0264(10) 0.0275(10) 0.0136(8) -0.0125(8) -0.0095(8)
C223 0.0256(9) 0.0174(9) 0.0328(10) 0.0026(8) -0.0128(8) -0.0028(7)
C224 0.0196(8) 0.0199(8) 0.0217(9) -0.0004(7) -0.0052(7) -0.0017(7)
B2 0.0125(8) 0.0167(9) 0.0154(9) 0.0014(7) -0.0002(7) 0.0004(7)

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

# 10. MOLECULAR GEOMETRY

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

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Ti1     C11      2.3521(16)                    .       .                   yes
```

Ti1	C12	2.3901(16)	.	.	yes
Ti1	C13	2.3844(17)	.	.	yes
Ti1	C14	2.3739(17)	.	.	yes
Ti1	C15	2.3239(17)	.	.	yes
Ti1	C111	2.3287(18)	.	.	yes
Ti1	C112	2.3096(19)	.	.	yes
Ti1	C113	2.3197(18)	.	.	yes
Ti1	C114	2.3564(18)	.	.	yes
Ti1	C115	2.3908(16)	.	.	yes
C11	C12	1.427(2)	.	.	no
C11	C15	1.426(2)	.	.	no
C11	C16	1.495(2)	.	.	no
C12	C13	1.405(2)	.	.	no
C12	C17	1.498(3)	.	.	no
C13	C14	1.428(2)	.	.	no
C13	C18	1.502(3)	.	.	no
C14	C15	1.417(2)	.	.	no
C14	C19	1.492(3)	.	.	no
C15	C110	1.504(3)	.	.	no
C111	C112	1.417(3)	.	.	no
C111	C115	1.427(2)	.	.	no
C112	C113	1.401(3)	.	.	no
C113	C114	1.418(3)	.	.	no
C114	C115	1.411(2)	.	.	no
C115	C116	1.517(2)	.	.	no
C116	C117	1.544(3)	.	.	no
C116	C124	1.547(3)	.	.	no
C16	H16	0.9800	.	.	no
C16	H16'	0.9364	.	.	no
C16	H16"	1.0382	.	.	no
C117	C118	1.533(3)	.	.	no
C117	C122	1.536(3)	.	.	no
C17	H17"	0.9755	.	.	no
C17	H17	1.0156	.	.	no
C17	H17'	1.0525	.	.	no
C118	C119	1.534(3)	.	.	no
C18	H18	0.9806	.	.	no
C18	H18"	0.9494	.	.	no
C18	H18'	1.0319	.	.	no
C19	H19'	1.0315	.	.	no
C19	H19"	0.9864	.	.	no
C119	C125	1.532(3)	.	.	no
C119	C120	1.539(3)	.	.	no
C19	H19	0.9074	.	.	no
C120	C121	1.527(3)	.	.	no
C121	C122	1.535(3)	.	.	no
C121	C123	1.524(3)	.	.	no
C123	C124	1.534(3)	.	.	no
C124	C125	1.531(3)	.	.	no
C110	H110'	0.9616	.	.	no
C110	H110"	0.9506	.	.	no
C110	H110	1.0140	.	.	no
C111	H111	0.9748	.	.	no
C112	H112	0.9580	.	.	no
C113	H113	0.9899	.	.	no
C114	H114	0.9599	.	.	no
C116	H116	1.0063	.	.	no
C117	H117	0.9841	.	.	no
C118	H118'	0.9752	.	.	no
C118	H118	1.0547	.	.	no
C119	H119	0.9838	.	.	no

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 C120    H120'        0.9899                    .      .                 no
 C120    H120         0.9926                    .      .                 no
 C121    H121         1.0088                    .      .                 no
 C21     C22         1.403(2)                   .      .                 no
 C21     C26         1.400(2)                   .      .                 no
 C21     B2          1.644(2)                   .      .                 yes
 C22     C23         1.388(3)                   .      .                 no
 C122    H122'        0.9958                    .      .                 no
 C122    H122         1.0393                    .      .                 no
 C123    H123'        1.0207                    .      .                 no
 C23     C24         1.381(3)                   .      .                 no
 C123    H123         0.9836                    .      .                 no
 C24     C25         1.381(3)                   .      .                 no
 C124    H124         0.9428                    .      .                 no
 C125    H125         1.0144                    .      .                 no
 C125    H125'        0.9886                    .      .                 no
 C25     C26         1.388(3)                   .      .                 no
 C27     C28         1.405(2)                   .      .                 no
 C27     B2          1.636(2)                   .      .                 yes
 C27     C212        1.396(2)                   .      .                 no
 C28     C29         1.391(2)                   .      .                 no
 C29     C210        1.384(3)                   .      .                 no
 C22     H22          0.9544                    .      .                 no
 C23     H23          0.9280                    .      .                 no
 C24     H24          0.9997                    .      .                 no
 C25     H25          0.9606                    .      .                 no
 C26     H26          0.8987                    .      .                 no
 C28     H28          0.9059                    .      .                 no
 C29     H29          0.9484                    .      .                 no
 C210    C211        1.385(3)                   .      .                 no
 C211    C212        1.388(3)                   .      .                 no
 C213    C218        1.409(2)                   .      .                 no
 C213    C214        1.403(2)                   .      .                 no
 C213    B2          1.644(2)                   .      .                 yes
 C214    C215        1.388(2)                   .      .                 no
 C215    C216        1.403(2)                   .      .                 no
 C216    C217        1.389(3)                   .      .                 no
 C217    C218        1.387(2)                   .      .                 no
 C219    C220        1.405(2)                   .      .                 no
 C219    C224        1.406(2)                   .      .                 no
 C219    B2          1.642(2)                   .      .                 yes
 C220    C221        1.388(3)                   .      .                 no
 C221    C222        1.385(3)                   .      .                 no
 C222    C223        1.387(3)                   .      .                 no
 C223    C224        1.386(3)                   .      .                 no
 C210    H210         0.9541                    .      .                 no
 C211    H211         0.9050                    .      .                 no
 C212    H212         0.9938                    .      .                 no
 C214    H214         1.0209                    .      .                 no
 C215    H215         1.0196                    .      .                 no
 C216    H216         0.9386                    .      .                 no
 C217    H217         0.9442                    .      .                 no
 C218    H218         0.9248                    .      .                 no
 C220    H220         1.0137                    .      .                 no
 C221    H221         0.9564                    .      .                 no
 C222    H222         0.9650                    .      .                 no
 C223    H223         1.0026                    .      .                 no
 C224    H224         0.9547                    .      .                 no

loop_
_geom_angle_atom_site_label_1
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_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
 C11     Ti1     C12        35.00(6)              .       .       .           yes
 C11     Ti1     C13        57.95(6)              .       .       .           yes
 C11     Ti1     C14        58.29(6)              .       .       .           yes
 C11     Ti1     C15        35.49(6)              .       .       .           yes
 C11     Ti1     C111      162.80(6)              .       .       .           yes
 C11     Ti1     C112      155.26(6)              .       .       .           yes
 C11     Ti1     C113      138.58(6)              .       .       .           yes
 C11     Ti1     C114      134.33(6)              .       .       .           yes
 C11     Ti1     C115      145.36(6)              .       .       .           yes
 C12     Ti1     C13        34.22(6)              .       .       .           yes
 C12     Ti1     C14        57.64(6)              .       .       .           yes
 C12     Ti1     C15        58.40(6)              .       .       .           yes
 C12     Ti1     C111      150.28(6)              .       .       .           yes
 C12     Ti1     C112      120.31(6)              .       .       .           yes
 C12     Ti1     C113      113.75(6)              .       .       .           yes
 C12     Ti1     C114      134.37(6)              .       .       .           yes
 C12     Ti1     C115      168.81(6)              .       .       .           yes
 C13     Ti1     C14        34.92(6)              .       .       .           yes
 C13     Ti1     C15        58.38(6)              .       .       .           yes
 C13     Ti1     C111      137.48(6)              .       .       .           yes
 C13     Ti1     C112      102.30(6)              .       .       .           yes
 C13     Ti1     C113       82.57(6)              .       .       .           yes
 C13     Ti1     C114      100.44(6)              .       .       .           yes
 C13     Ti1     C115      134.98(6)              .       .       .           yes
 C14     Ti1     C15        35.09(6)              .       .       .           yes
 C14     Ti1     C111      137.85(6)              .       .       .           yes
 C14     Ti1     C112      115.38(6)              .       .       .           yes
 C14     Ti1     C113       82.56(6)              .       .       .           yes
 C14     Ti1     C114       80.94(6)              .       .       .           yes
 C14     Ti1     C115      111.81(6)              .       .       .           yes
 C15     Ti1     C111      150.94(6)              .       .       .           yes
 C15     Ti1     C112      149.39(7)              .       .       .           yes
 C15     Ti1     C113      114.47(7)              .       .       .           yes
 C15     Ti1     C114       99.04(6)              .       .       .           yes
 C15     Ti1     C115      115.87(6)              .       .       .           yes
 C111    Ti1     C112       35.56(6)              .       .       .           yes
 C111    Ti1     C113       58.60(6)              .       .       .           yes
 C111    Ti1     C114       58.18(6)              .       .       .           yes
 C111    Ti1     C115       35.17(6)              .       .       .           yes
 C112    Ti1     C113       35.23(7)              .       .       .           yes
 C112    Ti1     C114       58.66(6)              .       .       .           yes
 C112    Ti1     C115       58.82(6)              .       .       .           yes
 C113    Ti1     C114       35.29(6)              .       .       .           yes
 C113    Ti1     C115       58.36(6)              .       .       .           yes
 C114    Ti1     C115       34.58(6)              .       .       .           yes
 Ti1     C11     C12        73.95(9)              .       .       .           yes
 Ti1     C11     C15        71.17(9)              .       .       .           yes
 Ti1     C11     C16      128.40(12)              .       .       .           yes
 C12     C11     C15      107.53(15)              .       .       .           no
 C12     C11     C16      126.03(15)              .       .       .           no
 C15     C11     C16      125.63(15)              .       .       .           no
 Ti1     C12     C11        71.05(9)              .       .       .           yes
 Ti1     C12     C13        72.67(10)             .       .       .           yes
 Ti1     C12     C17      128.58(12)              .       .       .           yes
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C11	C12	C13	108.29(14)	.	.	.	no
C11	C12	C17	126.93(16)	.	.	.	no
C13	C12	C17	124.26(16)	.	.	.	no
Ti1	C13	C12	73.11(10)	.	.	.	yes
Ti1	C13	C14	72.13(10)	.	.	.	yes
Ti1	C13	C18	126.55(12)	.	.	.	yes
C12	C13	C14	108.32(14)	.	.	.	no
C12	C13	C18	123.78(16)	.	.	.	no
C14	C13	C18	127.46(15)	.	.	.	no
Ti1	C14	C13	72.94(10)	.	.	.	yes
Ti1	C14	C15	70.53(10)	.	.	.	yes
Ti1	C14	C19	128.69(13)	.	.	.	yes
C13	C14	C15	107.68(15)	.	.	.	no
C13	C14	C19	125.43(15)	.	.	.	no
C15	C14	C19	126.34(16)	.	.	.	no
Ti1	C15	C11	73.33(9)	.	.	.	yes
Ti1	C15	C14	74.38(10)	.	.	.	yes
Ti1	C15	C110	121.36(13)	.	.	.	yes
C11	C15	C14	108.13(15)	.	.	.	no
C11	C15	C110	125.81(16)	.	.	.	no
C14	C15	C110	125.95(16)	.	.	.	no
Ti1	C111	C112	71.48(10)	.	.	.	yes
Ti1	C111	C115	74.79(10)	.	.	.	yes
C112	C111	C115	108.60(16)	.	.	.	no
Ti1	C112	C111	72.96(10)	.	.	.	yes
Ti1	C112	C113	72.78(11)	.	.	.	yes
C111	C112	C113	107.67(16)	.	.	.	no
Ti1	C113	C112	71.99(11)	.	.	.	yes
Ti1	C113	C114	73.77(10)	.	.	.	yes
C112	C113	C114	108.37(16)	.	.	.	no
Ti1	C114	C113	70.94(10)	.	.	.	yes
Ti1	C114	C115	74.04(10)	.	.	.	yes
C113	C114	C115	108.59(16)	.	.	.	no
Ti1	C115	C111	70.04(9)	.	.	.	yes
Ti1	C115	C114	71.38(10)	.	.	.	yes
Ti1	C115	C116	123.06(11)	.	.	.	yes
C111	C115	C114	106.74(15)	.	.	.	no
C111	C115	C116	126.64(15)	.	.	.	no
C114	C115	C116	126.62(15)	.	.	.	no
C115	C116	C117	113.50(15)	.	.	.	no
C115	C116	C124	111.97(14)	.	.	.	no
C117	C116	C124	108.42(14)	.	.	.	no
H16'	C16	H16"	106.42	.	.	.	no
C11	C16	H16"	108.37	.	.	.	no
C11	C16	H16	111.52	.	.	.	no
C11	C16	H16'	111.94	.	.	.	no
H16	C16	H16'	106.65	.	.	.	no
H16	C16	H16"	111.86	.	.	.	no
C116	C117	C122	108.67(16)	.	.	.	no
C116	C117	C118	110.89(15)	.	.	.	no
C12	C17	H17	108.41	.	.	.	no
C12	C17	H17'	113.92	.	.	.	no
C12	C17	H17"	109.93	.	.	.	no
H17	C17	H17'	108.95	.	.	.	no
H17	C17	H17"	106.28	.	.	.	no
H17'	C17	H17"	109.07	.	.	.	no
C118	C117	C122	108.75(15)	.	.	.	no
C13	C18	H18'	109.53	.	.	.	no
C13	C18	H18"	104.18	.	.	.	no
C13	C18	H18	114.64	.	.	.	no
C117	C118	C119	109.89(16)	.	.	.	no

H18'	C18	H18"	112.50	.	.	.	no
H18	C18	H18"	110.72	.	.	.	no
H18	C18	H18'	105.46	.	.	.	no
C120	C119	C125	109.43(15)	.	.	.	no
C118	C119	C125	108.56(15)	.	.	.	no
H19'	C19	H19"	112.09	.	.	.	no
H19	C19	H19'	107.19	.	.	.	no
H19	C19	H19"	107.14	.	.	.	no
C118	C119	C120	109.65(15)	.	.	.	no
C14	C19	H19	108.70	.	.	.	no
C14	C19	H19'	112.77	.	.	.	no
C14	C19	H19"	108.74	.	.	.	no
C119	C120	C121	109.44(14)	.	.	.	no
C122	C121	C123	109.09(15)	.	.	.	no
C120	C121	C123	109.71(16)	.	.	.	no
C120	C121	C122	109.48(16)	.	.	.	no
C117	C122	C121	110.05(15)	.	.	.	no
C121	C123	C124	110.04(15)	.	.	.	no
C116	C124	C123	108.80(14)	.	.	.	no
C116	C124	C125	109.88(15)	.	.	.	no
C123	C124	C125	109.42(15)	.	.	.	no
C119	C125	C124	110.31(14)	.	.	.	no
C15	C110	H110'	113.81	.	.	.	no
C15	C110	H110"	111.62	.	.	.	no
C15	C110	H110	111.85	.	.	.	no
H110'	C110	H110"	105.25	.	.	.	no
H110'	C110	H110	101.84	.	.	.	no
H110"	C110	H110	111.95	.	.	.	no
Ti1	C111	H111	119.48	.	.	.	no
C112	C111	H111	126.91	.	.	.	no
C115	C111	H111	124.49	.	.	.	no
Ti1	C112	H112	120.02	.	.	.	no
C111	C112	H112	124.72	.	.	.	no
C113	C112	H112	127.61	.	.	.	no
Ti1	C113	H113	121.59	.	.	.	no
C112	C113	H113	125.07	.	.	.	no
C114	C113	H113	126.53	.	.	.	no
Ti1	C114	H114	123.56	.	.	.	no
C113	C114	H114	125.32	.	.	.	no
C115	C114	H114	126.01	.	.	.	no
C115	C116	H116	107.29	.	.	.	no
C117	C116	H116	109.65	.	.	.	no
C124	C116	H116	105.70	.	.	.	no
C116	C117	H117	110.96	.	.	.	no
C118	C117	H117	109.55	.	.	.	no
C122	C117	H117	107.95	.	.	.	no
C117	C118	H118'	107.76	.	.	.	no
C117	C118	H118	108.21	.	.	.	no
C119	C118	H118'	111.95	.	.	.	no
C119	C118	H118	111.57	.	.	.	no
H118'	C118	H118	107.30	.	.	.	no
C118	C119	H119	109.71	.	.	.	no
C120	C119	H119	109.41	.	.	.	no
C125	C119	H119	110.08	.	.	.	no
C119	C120	H120'	109.84	.	.	.	no
C119	C120	H120	109.91	.	.	.	no
C121	C120	H120'	111.03	.	.	.	no
C121	C120	H120	107.96	.	.	.	no
H120'	C120	H120	108.64	.	.	.	no
C120	C121	H121	112.04	.	.	.	no
C122	C121	H121	108.38	.	.	.	no

C123	C121	H121	108.09	.	.	.	no
C22	C21	C26	115.68(15)	.	.	.	no
C22	C21	B2	120.55(14)	.	.	.	yes
C26	C21	B2	123.30(14)	.	.	.	yes
C117	C122	H122'	113.17	.	.	.	no
C117	C122	H122	108.44	.	.	.	no
C121	C122	H122'	109.57	.	.	.	no
C21	C22	C23	122.37(16)	.	.	.	no
C121	C122	H122	109.80	.	.	.	no
H122'	C122	H122	105.70	.	.	.	no
C124	C123	H123'	108.53	.	.	.	no
C121	C123	H123'	110.74	.	.	.	no
C124	C123	H123	111.14	.	.	.	no
H123'	C123	H123	106.80	.	.	.	no
C121	C123	H123	109.55	.	.	.	no
C22	C23	C24	120.07(17)	.	.	.	no
C116	C124	H124	111.11	.	.	.	no
C23	C24	C25	119.31(17)	.	.	.	no
C123	C124	H124	108.62	.	.	.	no
C125	C124	H124	108.97	.	.	.	no
H125'	C125	H125	110.48	.	.	.	no
C119	C125	H125'	107.82	.	.	.	no
C119	C125	H125	107.25	.	.	.	no
C124	C125	H125'	110.53	.	.	.	no
C124	C125	H125	110.36	.	.	.	no
C24	C25	C26	120.14(17)	.	.	.	no
C21	C26	C25	122.42(16)	.	.	.	no
C28	C27	C212	115.33(15)	.	.	.	no
C28	C27	B2	122.73(14)	.	.	.	yes
C212	C27	B2	121.52(14)	.	.	.	yes
C27	C28	C29	122.31(16)	.	.	.	no
C28	C29	C210	120.47(16)	.	.	.	no
C21	C22	H22	118.51	.	.	.	no
C23	C22	H22	119.12	.	.	.	no
C22	C23	H23	121.23	.	.	.	no
C24	C23	H23	118.62	.	.	.	no
C23	C24	H24	120.51	.	.	.	no
C25	C24	H24	120.18	.	.	.	no
C24	C25	H25	123.03	.	.	.	no
C26	C25	H25	116.83	.	.	.	no
C21	C26	H26	118.98	.	.	.	no
C25	C26	H26	118.44	.	.	.	no
C29	C28	H28	117.48	.	.	.	no
C27	C28	H28	120.21	.	.	.	no
C28	C29	H29	119.78	.	.	.	no
C210	C29	H29	119.75	.	.	.	no
C29	C210	C211	118.80(16)	.	.	.	no
C210	C211	C212	120.03(17)	.	.	.	no
C27	C212	C211	123.05(16)	.	.	.	no
C214	C213	C218	115.41(15)	.	.	.	no
C218	C213	B2	124.22(14)	.	.	.	yes
C214	C213	B2	119.76(14)	.	.	.	yes
C213	C214	C215	122.90(15)	.	.	.	no
C214	C215	C216	119.84(16)	.	.	.	no
C215	C216	C217	118.82(16)	.	.	.	no
C216	C217	C218	120.27(16)	.	.	.	no
C213	C218	C217	122.71(16)	.	.	.	no
C220	C219	B2	122.00(14)	.	.	.	yes
C220	C219	C224	115.34(15)	.	.	.	no
C224	C219	B2	122.26(14)	.	.	.	yes
C219	C220	C221	122.20(17)	.	.	.	no

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 C220    C221    C222     120.75(18)              .       .       .          no
 C221    C222    C223     118.72(18)              .       .       .          no
 C222    C223    C224     120.16(17)              .       .       .          no
 C219    C224    C223     122.83(17)              .       .       .          no
 C29     C210    H210         120.61              .       .       .          no
 C211    C210    H210         120.45              .       .       .          no
 C212    C211    H211         120.20              .       .       .          no
 C210    C211    H211         119.67              .       .       .          no
 C27     C212    H212         118.18              .       .       .          no
 C211    C212    H212         118.77              .       .       .          no
 C213    C214    H214         120.63              .       .       .          no
 C215    C214    H214         116.44              .       .       .          no
 C216    C215    H215         121.97              .       .       .          no
 C214    C215    H215         118.07              .       .       .          no
 C215    C216    H216         119.21              .       .       .          no
 C217    C216    H216         121.66              .       .       .          no
 C218    C217    H217         120.97              .       .       .          no
 C216    C217    H217         118.75              .       .       .          no
 C213    C218    H218         118.62              .       .       .          no
 C217    C218    H218         118.66              .       .       .          no
 C219    C220    H220         118.30              .       .       .          no
 C221    C220    H220         119.49              .       .       .          no
 C222    C221    H221         119.75              .       .       .          no
 C220    C221    H221         119.46              .       .       .          no
 C221    C222    H222         120.25              .       .       .          no
 C223    C222    H222         121.01              .       .       .          no
 C222    C223    H223         123.92              .       .       .          no
 C224    C223    H223         115.92              .       .       .          no
 C223    C224    H224         117.28              .       .       .          no
 C219    C224    H224         119.89              .       .       .          no
 C21     B2      C213     100.42(12)              .       .       .          yes
 C21     B2      C219     112.93(13)              .       .       .          yes
 C27     B2      C219     103.87(13)              .       .       .          yes
 C213    B2      C219     114.01(13)              .       .       .          yes
 C27     B2      C213     111.78(13)              .       .       .          yes
 C21     B2      C27      114.25(13)              .       .       .          yes

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
 C12     Ti1     C11     C15     -115.42(14)     .       .       .       .   no
 C12     Ti1     C11     C16      123.57(19)     .       .       .       .   no
 C13     Ti1     C11     C12       36.23(10)     .       .       .       .   no
 C13     Ti1     C11     C15      -79.20(11)     .       .       .       .   no
 C13     Ti1     C11     C16      159.80(17)     .       .       .       .   no
 C14     Ti1     C11     C12       77.61(11)     .       .       .       .   no
 C14     Ti1     C11     C15      -37.81(10)     .       .       .       .   no
 C14     Ti1     C11     C16     -158.82(17)     .       .       .       .   no
 C15     Ti1     C11     C12      115.42(14)     .       .       .       .   no
 C15     Ti1     C11     C16     -121.01(19)     .       .       .       .   no
 C112    Ti1     C11     C12         -4.5(2)     .       .       .       .   no
 C112    Ti1     C11     C15     -119.91(16)     .       .       .       .   no
 C112    Ti1     C11     C16      119.08(18)     .       .       .       .   no
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C113	Ti1	C11	C12	56.14(14)	.	.	.	.	no
C113	Ti1	C11	C15	-59.28(14)	.	.	.	.	no
C113	Ti1	C11	C16	179.71(13)	.	.	.	.	no
C114	Ti1	C11	C12	108.01(11)	.	.	.	.	no
C114	Ti1	C11	C15	-7.42(14)	.	.	.	.	no
C114	Ti1	C11	C16	-128.42(15)	.	.	.	.	no
C115	Ti1	C11	C12	160.35(11)	.	.	.	.	no
C115	Ti1	C11	C15	44.93(15)	.	.	.	.	no
C115	Ti1	C11	C16	-76.07(18)	.	.	.	.	no
C11	Ti1	C12	C13	117.05(14)	.	.	.	.	no
C11	Ti1	C12	C17	-122.6(2)	.	.	.	.	no
C13	Ti1	C12	C11	-117.05(14)	.	.	.	.	no
C13	Ti1	C12	C17	120.4(2)	.	.	.	.	no
C14	Ti1	C12	C11	-79.63(10)	.	.	.	.	no
C14	Ti1	C12	C13	37.42(9)	.	.	.	.	no
C14	Ti1	C12	C17	157.78(18)	.	.	.	.	no
C15	Ti1	C12	C11	-38.00(10)	.	.	.	.	no
C15	Ti1	C12	C13	79.04(11)	.	.	.	.	no
C15	Ti1	C12	C17	-160.59(18)	.	.	.	.	no
C111	Ti1	C12	C11	149.06(13)	.	.	.	.	no
C111	Ti1	C12	C13	-93.90(15)	.	.	.	.	no
C111	Ti1	C12	C17	26.5(2)	.	.	.	.	no
C112	Ti1	C12	C11	177.82(10)	.	.	.	.	no
C112	Ti1	C12	C13	-65.13(11)	.	.	.	.	no
C112	Ti1	C12	C17	55.24(18)	.	.	.	.	no
C113	Ti1	C12	C11	-143.11(10)	.	.	.	.	no
C113	Ti1	C12	C13	-26.07(12)	.	.	.	.	no
C113	Ti1	C12	C17	94.30(17)	.	.	.	.	no
C114	Ti1	C12	C11	-107.90(12)	.	.	.	.	no
C114	Ti1	C12	C13	9.14(14)	.	.	.	.	no
C114	Ti1	C12	C17	129.51(16)	.	.	.	.	no
C11	Ti1	C13	C12	-37.07(9)	.	.	.	.	no
C11	Ti1	C13	C14	79.24(10)	.	.	.	.	no
C11	Ti1	C13	C18	-156.95(17)	.	.	.	.	no
C12	Ti1	C13	C14	116.30(14)	.	.	.	.	no
C12	Ti1	C13	C18	-119.88(19)	.	.	.	.	no
C14	Ti1	C13	C12	-116.30(14)	.	.	.	.	no
C14	Ti1	C13	C18	123.82(19)	.	.	.	.	no
C15	Ti1	C13	C12	-79.11(11)	.	.	.	.	no
C15	Ti1	C13	C14	37.19(10)	.	.	.	.	no
C15	Ti1	C13	C18	161.00(17)	.	.	.	.	no
C111	Ti1	C13	C12	132.95(11)	.	.	.	.	no
C111	Ti1	C13	C14	-110.75(11)	.	.	.	.	no
C111	Ti1	C13	C18	13.07(19)	.	.	.	.	no
C112	Ti1	C13	C12	126.71(10)	.	.	.	.	no
C112	Ti1	C13	C14	-116.99(10)	.	.	.	.	no
C112	Ti1	C13	C18	6.83(16)	.	.	.	.	no
C113	Ti1	C13	C12	156.07(11)	.	.	.	.	no
C113	Ti1	C13	C14	-87.63(10)	.	.	.	.	no
C113	Ti1	C13	C18	36.19(15)	.	.	.	.	no
C114	Ti1	C13	C12	-173.37(10)	.	.	.	.	no
C114	Ti1	C13	C14	-57.07(11)	.	.	.	.	no
C114	Ti1	C13	C18	66.75(16)	.	.	.	.	no
C115	Ti1	C13	C12	-175.37(9)	.	.	.	.	no
C115	Ti1	C13	C14	-59.07(13)	.	.	.	.	no
C115	Ti1	C13	C18	64.75(17)	.	.	.	.	no
C11	Ti1	C14	C13	-78.20(10)	.	.	.	.	no
C11	Ti1	C14	C15	38.25(10)	.	.	.	.	no
C11	Ti1	C14	C19	159.72(18)	.	.	.	.	no
C12	Ti1	C14	C13	-36.65(10)	.	.	.	.	no
C12	Ti1	C14	C15	79.80(11)	.	.	.	.	no

C12	Ti1	C14	C19	-158.73(18)	.	.	.	.	no
C13	Ti1	C14	C15	116.45(14)	.	.	.	.	no
C13	Ti1	C14	C19	-122.08(19)	.	.	.	.	no
C15	Ti1	C14	C13	-116.45(14)	.	.	.	.	no
C15	Ti1	C14	C19	121.5(2)	.	.	.	.	no
C111	Ti1	C14	C13	109.65(12)	.	.	.	.	no
C111	Ti1	C14	C15	-133.90(11)	.	.	.	.	no
C111	Ti1	C14	C19	-12.4(2)	.	.	.	.	no
C112	Ti1	C14	C13	74.49(11)	.	.	.	.	no
C112	Ti1	C14	C15	-169.05(10)	.	.	.	.	no
C112	Ti1	C14	C19	-47.59(17)	.	.	.	.	no
C113	Ti1	C14	C13	87.67(10)	.	.	.	.	no
C113	Ti1	C14	C15	-155.88(11)	.	.	.	.	no
C113	Ti1	C14	C19	-34.42(15)	.	.	.	.	no
C114	Ti1	C14	C13	123.30(11)	.	.	.	.	no
C114	Ti1	C14	C15	-120.25(11)	.	.	.	.	no
C114	Ti1	C14	C19	1.22(15)	.	.	.	.	no
C115	Ti1	C14	C13	139.19(10)	.	.	.	.	no
C115	Ti1	C14	C15	-104.36(10)	.	.	.	.	no
C115	Ti1	C14	C19	17.11(17)	.	.	.	.	no
C11	Ti1	C15	C14	-114.89(14)	.	.	.	.	no
C11	Ti1	C15	C110	122.19(19)	.	.	.	.	no
C12	Ti1	C15	C11	37.46(10)	.	.	.	.	no
C12	Ti1	C15	C14	-77.43(11)	.	.	.	.	no
C12	Ti1	C15	C110	159.66(17)	.	.	.	.	no
C13	Ti1	C15	C11	77.89(10)	.	.	.	.	no
C13	Ti1	C15	C14	-37.01(10)	.	.	.	.	no
C13	Ti1	C15	C110	-159.92(17)	.	.	.	.	no
C14	Ti1	C15	C11	114.89(14)	.	.	.	.	no
C14	Ti1	C15	C110	-122.92(19)	.	.	.	.	no
C111	Ti1	C15	C11	-149.74(13)	.	.	.	.	no
C111	Ti1	C15	C14	95.37(16)	.	.	.	.	no
C111	Ti1	C15	C110	-27.6(2)	.	.	.	.	no
C112	Ti1	C15	C11	134.58(13)	.	.	.	.	no
C112	Ti1	C15	C14	19.69(17)	.	.	.	.	no
C112	Ti1	C15	C110	-103.23(18)	.	.	.	.	no
C113	Ti1	C15	C11	141.32(10)	.	.	.	.	no
C113	Ti1	C15	C14	26.43(12)	.	.	.	.	no
C113	Ti1	C15	C110	-96.48(15)	.	.	.	.	no
C114	Ti1	C15	C11	174.64(10)	.	.	.	.	no
C114	Ti1	C15	C14	59.75(11)	.	.	.	.	no
C114	Ti1	C15	C110	-63.17(16)	.	.	.	.	no
C115	Ti1	C15	C11	-153.51(9)	.	.	.	.	no
C115	Ti1	C15	C14	91.61(11)	.	.	.	.	no
C115	Ti1	C15	C110	-31.31(17)	.	.	.	.	no
C12	Ti1	C111	C112	45.59(18)	.	.	.	.	no
C12	Ti1	C111	C115	161.68(12)	.	.	.	.	no
C13	Ti1	C111	C112	-10.53(15)	.	.	.	.	no
C13	Ti1	C111	C115	105.56(12)	.	.	.	.	no
C14	Ti1	C111	C112	-63.44(14)	.	.	.	.	no
C14	Ti1	C111	C115	52.64(14)	.	.	.	.	no
C15	Ti1	C111	C112	-121.96(14)	.	.	.	.	no
C15	Ti1	C111	C115	-5.88(19)	.	.	.	.	no
C112	Ti1	C111	C115	116.08(15)	.	.	.	.	no
C113	Ti1	C111	C112	-37.66(10)	.	.	.	.	no
C113	Ti1	C111	C115	78.42(11)	.	.	.	.	no
C114	Ti1	C111	C112	-79.36(11)	.	.	.	.	no
C114	Ti1	C111	C115	36.72(10)	.	.	.	.	no
C115	Ti1	C111	C112	-116.08(15)	.	.	.	.	no
C11	Ti1	C112	C111	-152.79(14)	.	.	.	.	no
C11	Ti1	C112	C113	91.90(17)	.	.	.	.	no

C12	Ti1	C112	C111	−155.78(10)	.	.	.	.	no
C12	Ti1	C112	C113	88.92(12)	.	.	.	.	no
C13	Ti1	C112	C111	172.74(10)	.	.	.	.	no
C13	Ti1	C112	C113	57.43(11)	.	.	.	.	no
C14	Ti1	C112	C111	138.37(10)	.	.	.	.	no
C14	Ti1	C112	C113	23.06(12)	.	.	.	.	no
C15	Ti1	C112	C111	125.99(13)	.	.	.	.	no
C15	Ti1	C112	C113	10.68(18)	.	.	.	.	no
C111	Ti1	C112	C113	−115.31(15)	.	.	.	.	no
C113	Ti1	C112	C111	115.31(15)	.	.	.	.	no
C114	Ti1	C112	C111	77.90(11)	.	.	.	.	no
C114	Ti1	C112	C113	−37.41(10)	.	.	.	.	no
C115	Ti1	C112	C111	37.21(10)	.	.	.	.	no
C115	Ti1	C112	C113	−78.10(11)	.	.	.	.	no
C11	Ti1	C113	C112	−140.79(11)	.	.	.	.	no
C11	Ti1	C113	C114	103.12(12)	.	.	.	.	no
C12	Ti1	C113	C112	−109.43(11)	.	.	.	.	no
C12	Ti1	C113	C114	134.48(10)	.	.	.	.	no
C13	Ti1	C113	C112	−123.86(11)	.	.	.	.	no
C13	Ti1	C113	C114	120.05(11)	.	.	.	.	no
C14	Ti1	C113	C112	−159.09(11)	.	.	.	.	no
C14	Ti1	C113	C114	84.82(11)	.	.	.	.	no
C15	Ti1	C113	C112	−174.05(10)	.	.	.	.	no
C15	Ti1	C113	C114	69.86(12)	.	.	.	.	no
C111	Ti1	C113	C112	38.03(10)	.	.	.	.	no
C111	Ti1	C113	C114	−78.07(11)	.	.	.	.	no
C112	Ti1	C113	C114	−116.09(15)	.	.	.	.	no
C114	Ti1	C113	C112	116.09(15)	.	.	.	.	no
C115	Ti1	C113	C112	79.54(11)	.	.	.	.	no
C115	Ti1	C113	C114	−36.55(10)	.	.	.	.	no
C11	Ti1	C114	C113	−115.74(11)	.	.	.	.	no
C11	Ti1	C114	C115	127.55(11)	.	.	.	.	no
C12	Ti1	C114	C113	−66.00(13)	.	.	.	.	no
C12	Ti1	C114	C115	177.29(9)	.	.	.	.	no
C13	Ti1	C114	C113	−60.79(11)	.	.	.	.	no
C13	Ti1	C114	C115	−177.50(10)	.	.	.	.	no
C14	Ti1	C114	C113	−89.90(11)	.	.	.	.	no
C14	Ti1	C114	C115	153.39(11)	.	.	.	.	no
C15	Ti1	C114	C113	−120.09(11)	.	.	.	.	no
C15	Ti1	C114	C115	123.20(10)	.	.	.	.	no
C111	Ti1	C114	C113	79.36(11)	.	.	.	.	no
C111	Ti1	C114	C115	−37.36(10)	.	.	.	.	no
C112	Ti1	C114	C113	37.35(10)	.	.	.	.	no
C112	Ti1	C114	C115	−79.37(11)	.	.	.	.	no
C113	Ti1	C114	C115	−116.72(15)	.	.	.	.	no
C115	Ti1	C114	C113	116.72(15)	.	.	.	.	no
C11	Ti1	C115	C111	149.72(11)	.	.	.	.	no
C11	Ti1	C115	C114	−93.81(14)	.	.	.	.	no
C11	Ti1	C115	C116	28.31(19)	.	.	.	.	no
C13	Ti1	C115	C111	−113.00(11)	.	.	.	.	no
C13	Ti1	C115	C114	3.48(14)	.	.	.	.	no
C13	Ti1	C115	C116	125.59(13)	.	.	.	.	no
C14	Ti1	C115	C111	−144.93(10)	.	.	.	.	no
C14	Ti1	C115	C114	−28.46(12)	.	.	.	.	no
C14	Ti1	C115	C116	93.66(14)	.	.	.	.	no
C15	Ti1	C115	C111	176.83(10)	.	.	.	.	no
C15	Ti1	C115	C114	−66.70(12)	.	.	.	.	no
C15	Ti1	C115	C116	55.42(15)	.	.	.	.	no
C111	Ti1	C115	C114	116.47(15)	.	.	.	.	no
C111	Ti1	C115	C116	−121.41(18)	.	.	.	.	no
C112	Ti1	C115	C111	−37.63(10)	.	.	.	.	no

C112	Ti1	C115	C114	78.85(11)	.	.	.	.	no
C112	Ti1	C115	C116	-159.04(16)	.	.	.	.	no
C113	Ti1	C115	C111	-79.16(11)	.	.	.	.	no
C113	Ti1	C115	C114	37.31(11)	.	.	.	.	no
C113	Ti1	C115	C116	159.43(16)	.	.	.	.	no
C114	Ti1	C115	C111	-116.47(15)	.	.	.	.	no
C114	Ti1	C115	C116	122.12(18)	.	.	.	.	no
C15	C11	C12	C13	0.14(19)	.	.	.	.	no
C15	C11	C12	C17	-171.78(17)	.	.	.	.	no
C16	C11	C12	C13	170.28(16)	.	.	.	.	no
C16	C11	C12	C17	-1.6(3)	.	.	.	.	no
C16	C11	C12	Ti1	-126.16(17)	.	.	.	.	no
C15	C11	C12	Ti1	63.70(11)	.	.	.	.	no
C12	C11	C15	Ti1	-65.54(11)	.	.	.	.	no
C12	C11	C15	C14	1.27(19)	.	.	.	.	no
C12	C11	C15	C110	177.46(17)	.	.	.	.	no
C16	C11	C15	Ti1	124.27(16)	.	.	.	.	no
C16	C11	C15	C14	-168.92(16)	.	.	.	.	no
Ti1	C11	C15	C14	66.81(12)	.	.	.	.	no
Ti1	C11	C15	C110	-117.00(18)	.	.	.	.	no
Ti1	C11	C12	C17	124.52(17)	.	.	.	.	no
Ti1	C11	C12	C13	-63.56(12)	.	.	.	.	no
C16	C11	C15	C110	7.3(3)	.	.	.	.	no
C11	C12	C13	C14	-1.49(19)	.	.	.	.	no
C17	C12	C13	Ti1	-125.30(17)	.	.	.	.	no
C17	C12	C13	C14	170.69(16)	.	.	.	.	no
C11	C12	C13	C18	-174.42(16)	.	.	.	.	no
Ti1	C12	C13	C14	-64.00(12)	.	.	.	.	no
Ti1	C12	C13	C18	123.07(17)	.	.	.	.	no
C11	C12	C13	Ti1	62.52(11)	.	.	.	.	no
C17	C12	C13	C18	-2.2(3)	.	.	.	.	no
C12	C13	C14	C19	-169.62(17)	.	.	.	.	no
C18	C13	C14	Ti1	-122.77(19)	.	.	.	.	no
C12	C13	C14	C15	2.3(2)	.	.	.	.	no
Ti1	C13	C14	C15	-62.37(12)	.	.	.	.	no
Ti1	C13	C14	C19	125.74(18)	.	.	.	.	no
C12	C13	C14	Ti1	64.64(12)	.	.	.	.	no
C18	C13	C14	C19	3.0(3)	.	.	.	.	no
C18	C13	C14	C15	174.87(17)	.	.	.	.	no
C13	C14	C15	Ti1	63.94(12)	.	.	.	.	no
C13	C14	C15	C11	-2.18(19)	.	.	.	.	no
C19	C14	C15	Ti1	-124.26(18)	.	.	.	.	no
C19	C14	C15	C11	169.62(17)	.	.	.	.	no
C13	C14	C15	C110	-178.36(17)	.	.	.	.	no
Ti1	C14	C15	C110	117.70(18)	.	.	.	.	no
Ti1	C14	C15	C11	-66.12(12)	.	.	.	.	no
C19	C14	C15	C110	-6.6(3)	.	.	.	.	no
Ti1	C111	C112	H112	-115.10	.	.	.	.	no
C115	C111	C112	H112	178.77	.	.	.	.	no
H111	C111	C112	Ti1	113.43	.	.	.	.	no
H111	C111	C112	C113	178.42	.	.	.	.	no
H111	C111	C112	H112	-1.67	.	.	.	.	no
H111	C111	C115	Ti1	-115.59	.	.	.	.	no
H111	C111	C115	C114	-177.95	.	.	.	.	no
H111	C111	C115	C116	1.35	.	.	.	.	no
Ti1	C112	C113	H113	-116.41	.	.	.	.	no
C111	C112	C113	H113	178.48	.	.	.	.	no
H112	C112	C113	Ti1	114.98	.	.	.	.	no
H112	C112	C113	C114	-179.71	.	.	.	.	no
H112	C112	C113	H113	-1.43	.	.	.	.	no
Ti1	C113	C114	H114	-118.16	.	.	.	.	no

C112	C113	C114	H114	177.68	.	.	.	.	no
H113	C113	C114	Ti1	117.60	.	.	.	.	no
H113	C113	C114	C115	-177.42	.	.	.	.	no
H113	C113	C114	H114	-0.56	.	.	.	.	no
H114	C114	C115	Ti1	120.19	.	.	.	.	no
H114	C114	C115	C111	-178.33	.	.	.	.	no
H114	C114	C115	C116	2.37	.	.	.	.	no
Ti1	C115	C116	H116	9.22	.	.	.	.	no
C111	C115	C116	H116	-79.43	.	.	.	.	no
C114	C115	C116	H116	99.73	.	.	.	.	no
C115	C116	C117	H117	55.09	.	.	.	.	no
C124	C116	C117	H117	-179.82	.	.	.	.	no
H116	C116	C117	C118	173.14	.	.	.	.	no
H116	C116	C117	C122	53.66	.	.	.	.	no
H116	C116	C117	H117	-64.88	.	.	.	.	no
C115	C116	C124	H124	-53.04	.	.	.	.	no
C117	C116	C124	H124	-179.02	.	.	.	.	no
H116	C116	C124	C123	-56.08	.	.	.	.	no
H116	C116	C124	C125	-175.85	.	.	.	.	no
H116	C116	C124	H124	63.47	.	.	.	.	no
C116	C117	C118	H118'	62.56	.	.	.	.	no
C116	C117	C118	H118	178.29	.	.	.	.	no
C122	C117	C118	H118'	-178.01	.	.	.	.	no
C122	C117	C118	H118	-62.29	.	.	.	.	no
H117	C117	C118	C119	177.53	.	.	.	.	no
H117	C117	C118	H118'	-60.24	.	.	.	.	no
H117	C117	C118	H118	55.48	.	.	.	.	no
C116	C117	C122	H122'	-62.13	.	.	.	.	no
C116	C117	C122	H122	-179.06	.	.	.	.	no
C118	C117	C122	H122'	177.07	.	.	.	.	no
C118	C117	C122	H122	60.14	.	.	.	.	no
H117	C117	C122	C121	-178.76	.	.	.	.	no
H117	C117	C122	H122'	58.29	.	.	.	.	no
H117	C117	C122	H122	-58.64	.	.	.	.	no
C117	C118	C119	H119	179.91	.	.	.	.	no
H118'	C118	C119	C120	-179.62	.	.	.	.	no
H118'	C118	C119	C125	-60.12	.	.	.	.	no
H118'	C118	C119	H119	60.20	.	.	.	.	no
H118	C118	C119	C120	60.11	.	.	.	.	no
H118	C118	C119	C125	179.61	.	.	.	.	no
H118	C118	C119	H119	-60.06	.	.	.	.	no
C118	C119	C120	H120'	-62.61	.	.	.	.	no
C118	C119	C120	H120	177.90	.	.	.	.	no
C125	C119	C120	H120'	178.42	.	.	.	.	no
C125	C119	C120	H120	58.94	.	.	.	.	no
H119	C119	C120	C121	179.87	.	.	.	.	no
H119	C119	C120	H120'	57.75	.	.	.	.	no
H119	C119	C120	H120	-61.74	.	.	.	.	no
C118	C119	C125	H125'	178.60	.	.	.	.	no
C118	C119	C125	H125	59.60	.	.	.	.	no
C120	C119	C125	H125'	-61.77	.	.	.	.	no
C120	C119	C125	H125	179.24	.	.	.	.	no
H119	C119	C125	C124	179.28	.	.	.	.	no
H119	C119	C125	H125'	58.50	.	.	.	.	no
H119	C119	C125	H125	-60.49	.	.	.	.	no
C119	C120	C121	H121	-179.80	.	.	.	.	no
H120'	C120	C121	C122	61.88	.	.	.	.	no
H120'	C120	C121	C123	-178.44	.	.	.	.	no
H120'	C120	C121	H121	-58.38	.	.	.	.	no
H120	C120	C121	C122	-179.13	.	.	.	.	no
H120	C120	C121	C123	-59.46	.	.	.	.	no

H120	C120	C121	H121	60.60	.	.	.	no
C120	C121	C122	H122'	-174.66	.	.	.	no
C120	C121	C122	H122	-58.99	.	.	.	no
C123	C121	C122	H122'	65.29	.	.	.	no
C123	C121	C122	H122	-179.04	.	.	.	no
H121	C121	C122	C117	-177.22	.	.	.	no
H121	C121	C122	H122'	-52.18	.	.	.	no
H121	C121	C122	H122	63.49	.	.	.	no
C120	C121	C123	H123'	59.90	.	.	.	no
C120	C121	C123	H123	177.44	.	.	.	no
C122	C121	C123	H123'	179.81	.	.	.	no
C122	C121	C123	H123	-62.65	.	.	.	no
H121	C121	C123	C124	177.47	.	.	.	no
H121	C121	C123	H123'	-62.54	.	.	.	no
H121	C121	C123	H123	55.00	.	.	.	no
B2	C21	C22	C23	-172.67(16)	.	.	.	no
C22	C21	C26	C25	1.2(2)	.	.	.	no
B2	C21	C26	C25	173.36(16)	.	.	.	no
C22	C21	B2	C27	-159.49(15)	.	.	.	no
C22	C21	B2	C213	80.73(17)	.	.	.	no
C22	C21	B2	C219	-41.1(2)	.	.	.	no
C26	C21	B2	C27	28.7(2)	.	.	.	no
C26	C21	B2	C213	-91.06(17)	.	.	.	no
C26	C21	B2	C219	147.14(15)	.	.	.	no
C26	C21	C22	C23	-0.3(2)	.	.	.	no
C21	C22	C23	C24	-0.8(3)	.	.	.	no
C22	C23	C24	C25	1.0(3)	.	.	.	no
H123	C123	C124	C116	60.42	.	.	.	no
H123	C123	C124	C125	-179.52	.	.	.	no
H123'	C123	C124	H124	56.48	.	.	.	no
C121	C123	C124	H124	177.80	.	.	.	no
H123'	C123	C124	C116	177.57	.	.	.	no
H123'	C123	C124	C125	-62.37	.	.	.	no
H123	C123	C124	H124	-60.67	.	.	.	no
H124	C124	C125	H125'	-58.08	.	.	.	no
H124	C124	C125	H125	64.43	.	.	.	no
H124	C124	C125	C119	-177.23	.	.	.	no
C116	C124	C125	H125'	179.97	.	.	.	no
C116	C124	C125	H125	-57.53	.	.	.	no
C123	C124	C125	H125'	60.56	.	.	.	no
C123	C124	C125	H125	-176.93	.	.	.	no
C23	C24	C25	C26	-0.1(3)	.	.	.	no
C24	C25	C26	C21	-1.1(3)	.	.	.	no
C212	C27	C28	C29	0.5(3)	.	.	.	no
B2	C27	C28	C29	173.07(16)	.	.	.	no
C28	C27	B2	C21	36.9(2)	.	.	.	no
C28	C27	B2	C213	150.12(16)	.	.	.	no
C28	C27	B2	C219	-86.51(18)	.	.	.	no
C212	C27	B2	C21	-150.93(15)	.	.	.	no
C212	C27	B2	C213	-37.7(2)	.	.	.	no
C212	C27	B2	C219	85.62(18)	.	.	.	no
C28	C27	C212	C211	0.5(3)	.	.	.	no
B2	C27	C212	C211	-172.22(16)	.	.	.	no
C27	C28	C29	C210	-0.7(3)	.	.	.	no
C28	C29	C210	C211	-0.2(3)	.	.	.	no
C29	C210	C211	C212	1.1(3)	.	.	.	no
C210	C211	C212	C27	-1.3(3)	.	.	.	no
C218	C213	B2	C219	21.3(2)	.	.	.	no
C214	C213	C218	C217	-2.0(2)	.	.	.	no
C214	C213	B2	C27	-50.6(2)	.	.	.	no
C214	C213	B2	C219	-168.05(14)	.	.	.	no

C218	C213	B2	C27	138.74(16)	.	.	.	.	no
C218	C213	C214	C215	1.1(2)	.	.	.	.	no
B2	C213	C214	C215	-170.38(15)	.	.	.	.	no
B2	C213	C218	C217	169.01(16)	.	.	.	.	no
C214	C213	B2	C21	70.92(17)	.	.	.	.	no
C218	C213	B2	C21	-99.71(17)	.	.	.	.	no
C213	C214	C215	C216	1.0(3)	.	.	.	.	no
C214	C215	C216	C217	-2.2(3)	.	.	.	.	no
C215	C216	C217	C218	1.3(3)	.	.	.	.	no
C216	C217	C218	C213	0.9(3)	.	.	.	.	no
C220	C219	C224	C223	-0.4(3)	.	.	.	.	no
B2	C219	C224	C223	-173.25(16)	.	.	.	.	no
B2	C219	C220	C221	172.90(17)	.	.	.	.	no
C224	C219	B2	C21	-29.0(2)	.	.	.	.	no
C224	C219	B2	C27	95.29(17)	.	.	.	.	no
C224	C219	B2	C213	-142.82(16)	.	.	.	.	no
C220	C219	B2	C21	158.61(15)	.	.	.	.	no
C220	C219	B2	C27	-77.08(18)	.	.	.	.	no
C220	C219	B2	C213	44.8(2)	.	.	.	.	no
C224	C219	C220	C221	0.0(3)	.	.	.	.	no
C219	C220	C221	C222	0.7(3)	.	.	.	.	no
C220	C221	C222	C223	-1.1(3)	.	.	.	.	no
C221	C222	C223	C224	0.8(3)	.	.	.	.	no
C222	C223	C224	C219	0.0(3)	.	.	.	.	no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
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Ti1	C214	3.6798(17)	.	1_455	no
Ti1	C215	2.6976(17)	.	1_455	no
Ti1	C216	2.6103(19)	.	1_455	no
Ti1	C217	3.5824(19)	.	1_455	no
Ti1	H116	3.2977	.	.	no
Ti1	H215	2.6961	.	1_455	no
Ti1	H216	2.5122	.	1_455	no
C11	C13	2.295(2)	.	.	no
C11	C14	2.302(2)	.	.	no
C11	C17	2.617(3)	.	.	no
C11	C110	2.608(3)	.	.	no
C11	C215	3.356(2)	.	1_455	no
C11	C216	3.282(2)	.	1_455	no
C12	C15	2.301(2)	.	.	no
C12	C223	3.391(3)	.	2_645	no
C12	C14	2.296(2)	.	.	no
C12	C215	3.427(2)	.	1_455	no
C12	C16	2.603(3)	.	.	no
C12	C18	2.564(3)	.	.	no
C13	C223	3.512(3)	.	2_645	no
C13	C15	2.297(2)	.	.	no
C13	C17	2.567(3)	.	.	no
C13	C11	2.295(2)	.	.	no
C13	C113	3.104(2)	.	.	no
C13	C19	2.595(3)	.	.	no
C14	C11	2.302(2)	.	.	no
C14	C114	3.070(2)	.	.	no
C14	C12	2.296(2)	.	.	no
C14	C18	2.627(3)	.	.	no

C14	C110	2.602(3)	.	.	no
C14	C113	3.097(2)	.	.	no
C15	C12	2.301(2)	.	.	no
C15	C13	2.297(2)	.	.	no
C15	C114	3.560(2)	.	.	no
C15	C19	2.596(3)	.	.	no
C15	C16	2.598(3)	.	.	no
C16	C215	3.465(3)	.	1_455	no
C16	C216	3.270(3)	.	1_455	no
C16	C23	3.567(3)	.	2_645	no
C17	C215	3.597(3)	.	1_455	no
C19	C29	3.534(3)	.	4_555	no
C19	C28	3.564(3)	.	4_555	no
C22	C111	3.446(2)	.	1_655	no
C22	C224	3.193(3)	.	.	no
C23	C111	3.475(3)	.	1_655	no
C23	C16	3.567(3)	.	2_655	no
C24	C112	3.520(3)	.	1_655	no
C26	C28	3.231(3)	.	.	no
C26	C110	3.568(3)	.	.	no
C26	C214	3.423(2)	.	.	no
C28	C19	3.564(3)	.	4_554	no
C28	C26	3.231(3)	.	.	no
C29	C19	3.534(3)	.	4_554	no
C110	C26	3.568(3)	.	.	no
C111	C22	3.446(2)	.	1_455	no
C11	H216	2.6588	.	1_455	no
C111	C125	3.521(2)	.	.	no
C111	C23	3.475(3)	.	1_455	no
C111	C217	3.290(3)	.	1_455	no
C111	C114	2.278(3)	.	.	no
C111	C215	3.313(2)	.	1_455	no
C111	C214	3.492(2)	.	1_455	no
C111	C218	3.488(2)	.	1_455	no
C11	H215	2.8099	.	1_455	no
C111	C113	2.275(3)	.	.	no
C111	C116	2.631(2)	.	.	no
C111	C216	3.188(3)	.	1_455	no
C112	C114	2.286(3)	.	.	no
C112	C115	2.309(2)	.	.	no
C12	H215	2.6644	.	1_455	no
C112	C24	3.520(3)	.	1_455	no
C113	C19	3.356(3)	.	.	no
C113	C115	2.297(2)	.	.	no
C113	C14	3.097(2)	.	.	no
C13	H113	2.9530	.	.	no
C113	C111	2.275(3)	.	.	no
C113	C13	3.104(2)	.	.	no
C113	C18	3.338(3)	.	.	no
C114	C111	2.278(3)	.	.	no
C14	H114	3.0360	.	.	no
C114	C116	2.617(3)	.	.	no
C14	H113	3.0899	.	.	no
C114	C14	3.070(2)	.	.	no
C114	C112	2.286(3)	.	.	no
C114	C19	3.158(3)	.	.	no
C114	C118	3.370(3)	.	.	no
C114	C15	3.560(2)	.	.	no
C115	C113	2.297(2)	.	.	no
C115	C112	2.309(2)	.	.	no
C15	H223	3.0764	.	2_645	no

C115	C216	3.527(2)	.	1_455	no
C16	H216	2.5506	.	1_455	no
C116	C120	3.569(2)	.	.	no
C16	H110'	2.9268	.	.	no
C16	H215	2.9547	.	1_455	no
C16	H17'	2.8769	.	.	no
C116	C217	3.450(3)	.	1_455	no
C17	H16'	3.0351	.	.	no
C17	H18	3.0621	.	.	no
C17	H215	2.6181	.	1_455	no
C17	H18"	3.0305	.	.	no
C17	H125'	3.0297	.	2_545	no
C118	C114	3.370(3)	.	.	no
C118	C123	3.533(3)	.	.	no
C18	H19'	2.9922	.	.	no
C18	H17"	2.9323	.	.	no
C18	H113	2.7846	.	.	no
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;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
 Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
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 Date of submission :  2009-09-28  11:59:44

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;
 Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
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The atoms of the solvent showed unrealistic displacement parameters when
allowed to vary anisotropically, suggesting dynamic disorder (dynamic means
that the smeared electron density is due to fluctuations of the atomic
positions within each unit cell). A subsequent difference Fourier synthesis
resulted in the location of most hydrogen atoms; the remaining hydrogen atoms
were generated by geometrical considerations. The hydrogen atom coordinates
and isotropic displacement parameters were refined, except those belonging to
the cyclohexane solvent molecules, which were allowed to ride on their carrier
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Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S. Gould, R.O. Isra\"el, & Smits, J.M.M. (1999). The DIRDIF99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

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Sheldrick, G.M. SHELXL97. Program for Crystal Structure Refinement. University of G\"ottingen, Germany, 1997.

Spek, A. L. (2003). J. Appl. Cryst. 36, 7--13.
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Fig. 1. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.
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_cell_length_b                         14.7326(6)
_cell_length_c                         15.9679(7)
_cell_angle_alpha                      78.727(1)
_cell_angle_beta                       69.475(1)
_cell_angle_gamma                      69.452(1)
_cell_volume                          2693.0(2)
_cell_formula_units_Z                  2

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      8144
_cell_measurement_theta_min        2.53
_cell_measurement_theta_max       28.99
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   8144 reflections after integration using the SAINT software
   package (Bruker, 2001).
;

_exptl_crystal_description       'platelet'
_exptl_crystal_colour            'blueisch-green'
_exptl_crystal_size_max           0.34
_exptl_crystal_size_mid           0.19
_exptl_crystal_size_min           0.055
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.199
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1054
_exptl_absorpt_coefficient_mu     0.204
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    'SADABS, (Bruker, 2001)'
_exptl_absorpt_correction_T_min   0.9160
_exptl_absorpt_correction_T_max   0.9889


#==============================================================================
```

```
# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method            'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2001)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              22352
_diffrn_reflns_av_R_equivalents    0.0349
_diffrn_reflns_av_sigmaI/netI      0.0634
_diffrn_reflns_limit_h_min         -15
_diffrn_reflns_limit_h_max         16
_diffrn_reflns_limit_k_min         -18
_diffrn_reflns_limit_k_max         18
_diffrn_reflns_limit_l_min         -20
_diffrn_reflns_limit_l_max         20
_diffrn_reflns_theta_min           2.53
_diffrn_reflns_theta_max           26.73
_diffrn_measured_fraction_theta_max    0.975
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.985

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

# number of unique reflections
```

```
_reflns_number_total              11141
_reflns_number_gt                 8030
_reflns_threshold_expression      I>2\s(I)


_computing_data_collection          'SMART (Bruker, 2001)'
_computing_cell_refinement          'SAINT-Plus (Bruker, 2001)'
_computing_data_reduction           'SAINT-Plus'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 2003)
;
_computing_publication_material      'PLATON (Spek, 2003)'

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

# 8. REFINEMENT DATA


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

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0903P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment       constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?

_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          11141
_refine_ls_number_parameters      911
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0816
_refine_ls_R_factor_gt            0.0569
_refine_ls_wR_factor_ref          0.1578
_refine_ls_wR_factor_gt           0.1466
_refine_ls_goodness_of_fit_ref    1.068
_refine_ls_restrained_S_all       1.068
```

```
_refine_ls_shift/su_max           0.019
_refine_ls_shift/su_mean          0.001
_refine_diff_density_max          0.943
_refine_diff_density_min         -0.557
_refine_diff_density_rms          0.064

_vrn_publ_code_frame_time_sec      10.0
_vrn_publ_code_meas_time_hour       8.5

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

# 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
Ti1 Ti Uani 0.12440(3) 0.26778(3) 0.28215(2) 1.000 0.0135(1) . .
O11 O Uani 0.14403(13) 0.19383(11) 0.16651(10) 1.000 0.0167(5) . .
O12 O Uani 0.26008(13) 0.31863(11) 0.17261(10) 1.000 0.0171(5) . .
C11 C Uani 0.2714(2) 0.12391(17) 0.31378(15) 1.000 0.0184(7) . .
C12 C Uani 0.2887(2) 0.20307(17) 0.33961(15) 1.000 0.0188(7) . .
C13 C Uani 0.1916(2) 0.24443(17) 0.41067(14) 1.000 0.0185(7) . .
C14 C Uani 0.1155(2) 0.18854(16) 0.43203(14) 1.000 0.0174(7) . .
C15 C Uani 0.1630(2) 0.11514(16) 0.37173(14) 1.000 0.0180(7) . .
C16 C Uani 0.3581(2) 0.05214(19) 0.24843(18) 1.000 0.0230(8) . .
C17 C Uani 0.3959(2) 0.2322(2) 0.30916(18) 1.000 0.0251(8) . .
C18 C Uani 0.1798(3) 0.3231(2) 0.46383(18) 1.000 0.0257(9) . .
C19 C Uani 0.0185(3) 0.1901(2) 0.51713(17) 1.000 0.0257(8) . .
C110 C Uani 0.1197(3) 0.02983(18) 0.38429(17) 1.000 0.0230(8) . .
C111 C Uani -0.0553(2) 0.34886(18) 0.24535(16) 1.000 0.0210(7) . .
C112 C Uani 0.0114(2) 0.41157(18) 0.22213(16) 1.000 0.0225(7) . .
C113 C Uani 0.0216(2) 0.43035(18) 0.30191(16) 1.000 0.0208(7) . .
C114 C Uani -0.03864(19) 0.37743(17) 0.37339(16) 1.000 0.0186(7) . .
C115 C Uani -0.08727(19) 0.32594(17) 0.33905(15) 1.000 0.0186(7) . .
C116 C Uani -0.1679(2) 0.26784(19) 0.39239(17) 1.000 0.0244(8) . .
C117 C Uani -0.2536(2) 0.31608(19) 0.47845(17) 1.000 0.0251(8) . .
C118 C Uani -0.3225(3) 0.2485(2) 0.5356(2) 1.000 0.0424(10) . .
C119 C Uani -0.3901(3) 0.2305(3) 0.4837(3) 1.000 0.0555(11) . .
C120 C Uani -0.4724(3) 0.3274(3) 0.4598(2) 1.000 0.0494(13) . .
C121 C Uani -0.4045(2) 0.3948(2) 0.40148(18) 1.000 0.0357(9) . .
C122 C Uani -0.3211(3) 0.3478(3) 0.3152(2) 1.000 0.0435(12) . .
C123 C Uani -0.2373(2) 0.2518(2) 0.3394(2) 1.000 0.0401(10) . .
C124 C Uani -0.3066(3) 0.1840(3) 0.3965(3) 1.000 0.0627(16) . .
C125 C Uani -0.3359(2) 0.41216(19) 0.45340(17) 1.000 0.0245(8) . .
C126 C Uani 0.1106(2) 0.10570(18) 0.17829(16) 1.000 0.0213(8) . .
C127 C Uani 0.1115(3) 0.0899(2) 0.08728(18) 1.000 0.0311(10) . .
C128 C Uani 0.1723(2) 0.15814(19) 0.02242(16) 1.000 0.0237(8) . .
C129 C Uani 0.1357(2) 0.24177(18) 0.07791(15) 1.000 0.0205(8) . .
C130 C Uani 0.3617(2) 0.25780(18) 0.10974(16) 1.000 0.0201(7) . .
C131 C Uani 0.4131(2) 0.32883(18) 0.04136(16) 1.000 0.0216(7) . .
C132 C Uani 0.3946(2) 0.40627(18) 0.10055(16) 1.000 0.0212(7) . .
C133 C Uani 0.2745(2) 0.41562(17) 0.16375(16) 1.000 0.0191(7) . .
```

```
H16 H Uiso 0.34568 0.06367 0.19362 1.00(3) 0.017(2) . .
H16' H Uiso 0.35871 -0.01146 0.27513 1.00(4) 0.037(2) . .
H16" H Uiso 0.43531 0.05657 0.23793 1.00(4) 0.038(3) . .
H17 H Uiso 0.38589 0.30183 0.28278 1.00(4) 0.034(2) . .
H17' H Uiso 0.46036 0.18780 0.26284 1.00(4) 0.034(2) . .
H17" H Uiso 0.42529 0.22275 0.35915 1.00(4) 0.027(2) . .
H18 H Uiso 0.21981 0.29699 0.50647 1.00(5) 0.075(3) . .
H18' H Uiso 0.10418 0.35228 0.50098 1.00(5) 0.057(3) . .
H18" H Uiso 0.20510 0.37490 0.42707 1.00(6) 0.095(4) . .
H19 H Uiso 0.04562 0.16025 0.56157 1.00(5) 0.048(3) . .
H19' H Uiso -0.03619 0.15885 0.51754 1.00(5) 0.048(3) . .
H19" H Uiso -0.02616 0.25199 0.53830 1.00(4) 0.027(2) . .
H110 H Uiso 0.12350 -0.00450 0.44352 1.00(4) 0.028(2) . .
H110' H Uiso 0.16997 -0.01755 0.33940 1.00(3) 0.021(2) . .
H110" H Uiso 0.04030 0.04842 0.38529 1.00(5) 0.061(3) . .
H111 H Uiso -0.07621 0.32659 0.20384 1.00(4) 0.024(2) . .
H112 H Uiso 0.04274 0.43646 0.16370 1.00(4) 0.030(2) . .
H113 H Uiso 0.06007 0.47293 0.30751 1.00(3) 0.0110(19) . .
H114 H Uiso -0.04899 0.37996 0.43483 1.00(3) 0.019(2) . .
H116 H Uiso -0.12234 0.20964 0.40933 1.00(3) 0.023(2) . .
H117 H Uiso -0.21092 0.32546 0.51370 1.00(4) 0.029(2) . .
H118 H Uiso -0.37326 0.27939 0.58918 1.00(4) 0.040(3) . .
H118' H Uiso -0.27045 0.18962 0.54998 1.00(4) 0.038(3) . .
H119 H Uiso -0.42929 0.18835 0.51309 1.00(5) 0.059(3) . .
H120 H Uiso -0.51700 0.31989 0.42728 1.00(5) 0.056(3) . .
H120' H Uiso -0.52564 0.35632 0.51821 1.00(4) 0.043(3) . .
H121 H Uiso -0.46284 0.45928 0.38690 1.00(4) 0.036(3) . .
H122 H Uiso -0.28039 0.39416 0.27596 1.00(4) 0.032(2) . .
H122' H Uiso -0.36269 0.33379 0.28023 1.00(4) 0.039(2) . .
H123 H Uiso -0.18665 0.22117 0.28597 1.00(4) 0.043(3) . .
H124 H Uiso -0.35472 0.16697 0.36989 1.00(6) 0.077(3) . .
H124' H Uiso -0.25799 0.12667 0.41846 1.00(4) 0.028(3) . .
H125 H Uiso -0.29435 0.45906 0.41833 1.00(3) 0.024(2) . .
H125' H Uiso -0.38676 0.44289 0.50597 1.00(3) 0.023(2) . .
H126 H Uiso 0.04068 0.11291 0.22370 1.00(3) 0.023(2) . .
H126' H Uiso 0.16922 0.04698 0.20090 1.00(4) 0.031(2) . .
H127 H Uiso 0.03898 0.11104 0.08560 1.00(4) 0.020(2) . .
H127' H Uiso 0.14671 0.02849 0.07574 1.00(4) 0.044(3) . .
H128 H Uiso 0.25540 0.12630 0.00719 1.00(4) 0.045(3) . .
H128' H Uiso 0.15094 0.17997 -0.02950 1.00(4) 0.033(2) . .
H129 H Uiso 0.17892 0.28613 0.06105 1.00(4) 0.023(2) . .
H129' H Uiso 0.05827 0.28197 0.08181 1.00(3) 0.008(2) . .
H130 H Uiso 0.33444 0.21731 0.08800 1.00(4) 0.032(2) . .
H130' H Uiso 0.41512 0.21750 0.14417 1.00(3) 0.014(2) . .
H131 H Uiso 0.37278 0.35474 -0.00446 1.00(4) 0.025(2) . .
H131' H Uiso 0.49297 0.29826 0.00954 1.00(4) 0.030(2) . .
H132 H Uiso 0.39322 0.47133 0.06440 1.00(4) 0.032(2) . .
H132' H Uiso 0.45077 0.38370 0.13766 1.00(3) 0.017(2) . .
H133 H Uiso 0.26171 0.43227 0.22402 1.00(3) 0.015(2) . .
H133' H Uiso 0.21626 0.46585 0.13978 1.00(3) 0.017(2) . .


C21 C Uani 0.27621(19) 0.80675(16) 0.07109(15) 1.000 0.0161(6) . .
C22 C Uani 0.3333(2) 0.83691(17) 0.11515(15) 1.000 0.0190(7) . .
C23 C Uani 0.4031(2) 0.89542(18) 0.07123(17) 1.000 0.0232(8) . .
C24 C Uani 0.4164(2) 0.92866(17) -0.01812(17) 1.000 0.0228(7) . .
C25 C Uani 0.3594(2) 0.90224(16) -0.06341(16) 1.000 0.0205(7) . .
C26 C Uani 0.2912(2) 0.84221(17) -0.01949(15) 1.000 0.0188(7) . .
C27 C Uani 0.06450(19) 0.83303(16) 0.16097(14) 1.000 0.0147(6) . .
C28 C Uani 0.0294(2) 0.87392(17) 0.24286(15) 1.000 0.0192(7) . .
```

```
C29 C Uani -0.0668(2) 0.95427(18) 0.26681(16) 1.000 0.0226(8) . .
C210 C Uani -0.1323(2) 0.99791(18) 0.20987(17) 1.000 0.0243(8) . .
C211 C Uani -0.0991(2) 0.96092(18) 0.12776(17) 1.000 0.0244(8) . .
C212 C Uani -0.0029(2) 0.88076(17) 0.10464(16) 1.000 0.0199(7) . .
C213 C Uani 0.1753(2) 0.67728(16) 0.06032(14) 1.000 0.0157(6) . .
C214 C Uani 0.0757(2) 0.65290(16) 0.07640(15) 1.000 0.0177(7) . .
C215 C Uani 0.0684(2) 0.59006(17) 0.02521(16) 1.000 0.0221(8) . .
C216 C Uani 0.1624(2) 0.54857(18) -0.04431(16) 1.000 0.0250(8) . .
C217 C Uani 0.2632(2) 0.56907(18) -0.06170(16) 1.000 0.0237(8) . .
C218 C Uani 0.2694(2) 0.63205(17) -0.01006(15) 1.000 0.0193(7) . .
C219 C Uani 0.2246(2) 0.67023(16) 0.20724(14) 1.000 0.0166(7) . .
C220 C Uani 0.3405(2) 0.62230(17) 0.20025(16) 1.000 0.0204(7) . .
C221 C Uani 0.3748(3) 0.55510(18) 0.26736(17) 1.000 0.0250(8) . .
C222 C Uani 0.2944(2) 0.53274(18) 0.34425(16) 1.000 0.0240(8) . .
C223 C Uani 0.1793(2) 0.57719(17) 0.35254(16) 1.000 0.0220(7) . .
C224 C Uani 0.1458(2) 0.64403(17) 0.28520(15) 1.000 0.0189(7) . .
B2 B Uani 0.1851(2) 0.74573(18) 0.12538(16) 1.000 0.0144(7) . .


H22 H Uiso 0.32616 0.81061 0.18094 1.00(3) 0.0136(19) . .
H23 H Uiso 0.43910 0.91296 0.10089 1.00(4) 0.032(2) . .
H24 H Uiso 0.46385 0.96591 -0.04811 1.00(4) 0.032(2) . .
H25 H Uiso 0.36362 0.92554 -0.12655 1.00(3) 0.0096(19) . .
H26 H Uiso 0.25442 0.82135 -0.05298 1.00(4) 0.017(2) . .
H28 H Uiso 0.07354 0.84860 0.28500 1.00(4) 0.024(2) . .
H29 H Uiso -0.08994 0.97510 0.32142 1.00(3) 0.021(2) . .
H210 H Uiso -0.19971 1.05158 0.22922 1.00(3) 0.025(2) . .
H211 H Uiso -0.13931 0.98359 0.08950 1.00(4) 0.030(2) . .
H212 H Uiso 0.01661 0.85822 0.04681 1.00(3) 0.0129(19) . .
H214 H Uiso 0.01151 0.68294 0.12418 1.00(4) 0.031(2) . .
H215 H Uiso 0.00062 0.57443 0.03799 1.00(4) 0.023(2) . .
H216 H Uiso 0.15454 0.51141 -0.08150 1.00(4) 0.022(2) . .
H217 H Uiso 0.32690 0.53633 -0.10871 1.00(4) 0.029(2) . .
H218 H Uiso 0.33940 0.64721 -0.02418 1.00(3) 0.015(2) . .
H220 H Uiso 0.39902 0.63273 0.14907 1.00(3) 0.020(2) . .
H221 H Uiso 0.44904 0.52498 0.25844 1.00(4) 0.025(2) . .
H222 H Uiso 0.32093 0.48533 0.39138 1.00(4) 0.033(2) . .
H223 H Uiso 0.12390 0.55883 0.40339 1.00(4) 0.039(2) . .
H224 H Uiso 0.06668 0.67200 0.28975 1.00(4) 0.026(2) . .


C31 C Uani 0.4041(4) 0.0551(4) 0.5158(4) 1.000 0.092(2) . .
C32 C Uani 0.4657(8) 0.0060(6) 0.5784(5) 1.000 0.135(4) . .
C33 C Uani 0.4400(10) 0.0047(6) 0.4420(8) 1.000 0.180(6) . .


H31 H Uiso 0.32138 0.06435 0.54578 1.000 0.1094 . .
H31' H Uiso 0.41445 0.12022 0.49639 1.000 0.1094 . .
H32 H Uiso 0.42887 0.04227 0.63283 1.000 0.1617 . .
H32' H Uiso 0.45473 -0.05898 0.59603 1.000 0.1617 . .
H33 H Uiso 0.42303 -0.05802 0.45759 1.000 0.2155 . .
H33' H Uiso 0.40587 0.04323 0.39487 1.000 0.2155 . .


C41 C Uani 0.3823(4) 0.2021(4) 0.7716(4) 1.000 0.102(2) . .
C42 C Uani 0.2395(5) 0.3737(4) 0.7461(5) 1.000 0.123(3) . .
C43 C Uani 0.3654(8) 0.2864(6) 0.8130(4) 1.000 0.153(4) . .
C44 C Uani 0.3426(6) 0.3669(4) 0.7537(5) 1.000 0.124(3) . .
C45 C Uani 0.2423(8) 0.3009(10) 0.6957(4) 1.000 0.198(6) . .
C46 C Uani 0.2747(7) 0.2092(7) 0.7468(5) 1.000 0.156(4) . .
```

```
H41 H Uiso 0.39924 0.14350 0.81318 1.000 0.1229 . .
H41' H Uiso 0.44905 0.19504 0.71662 1.000 0.1229 . .
H42 H Uiso 0.20908 0.43876 0.71699 1.000 0.1473 . .
H42' H Uiso 0.18533 0.36920 0.80707 1.000 0.1473 . .
H43 H Uiso 0.30050 0.29290 0.86925 1.000 0.1846 . .
H43' H Uiso 0.43503 0.28034 0.82772 1.000 0.1846 . .
H44 H Uiso 0.33795 0.42599 0.77738 1.000 0.1484 . .
H44' H Uiso 0.40298 0.35804 0.69486 1.000 0.1484 . .
H45 H Uiso 0.16609 0.31341 0.68895 1.000 0.2372 . .
H45' H Uiso 0.29898 0.30097 0.63521 1.000 0.2372 . .
H46 H Uiso 0.29215 0.15483 0.71092 1.000 0.1881 . .
H46' H Uiso 0.21080 0.20487 0.80205 1.000 0.1881 . .


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
Ti1 0.0135(2) 0.0133(2) 0.0132(2) -0.0020(2) -0.0045(2) -0.0028(2)
O11 0.0218(9) 0.0139(8) 0.0167(8) -0.0003(6) -0.0087(7) -0.0060(7)
O12 0.0163(8) 0.0134(8) 0.0200(8) -0.0048(6) -0.0028(7) -0.0038(7)
C11 0.0181(12) 0.0166(12) 0.0188(11) 0.0012(9) -0.0087(9) -0.0018(10)
C12 0.0185(12) 0.0198(12) 0.0198(11) 0.0018(9) -0.0116(10) -0.0042(10)
C13 0.0212(13) 0.0191(12) 0.0175(11) 0.0000(9) -0.0120(10) -0.0036(10)
C14 0.0208(12) 0.0179(12) 0.0138(10) 0.0020(9) -0.0087(9) -0.0048(10)
C15 0.0200(12) 0.0162(12) 0.0170(11) 0.0016(9) -0.0065(9) -0.0054(10)
C16 0.0223(14) 0.0181(13) 0.0244(13) -0.0032(10) -0.0054(11) -0.0024(11)
C17 0.0238(14) 0.0304(15) 0.0269(13) -0.0001(11) -0.0131(12) -0.0110(12)
C18 0.0361(17) 0.0239(14) 0.0222(13) -0.0051(11) -0.0146(12) -0.0078(13)
C19 0.0278(15) 0.0269(15) 0.0174(12) 0.0019(11) -0.0049(11) -0.0064(13)
C110 0.0312(16) 0.0170(13) 0.0215(12) 0.0000(10) -0.0086(11) -0.0085(12)
C111 0.0133(12) 0.0254(13) 0.0228(12) -0.0072(10) -0.0081(10) 0.0012(10)
C112 0.0174(12) 0.0238(13) 0.0193(12) 0.0019(10) -0.0060(10) 0.0005(11)
C113 0.0142(12) 0.0166(12) 0.0295(13) -0.0046(10) -0.0062(10) -0.0013(10)
C114 0.0142(12) 0.0185(12) 0.0202(12) -0.0065(9) -0.0053(9) 0.0011(10)
C115 0.0117(11) 0.0175(12) 0.0241(12) -0.0062(9) -0.0049(9) 0.0003(9)
C116 0.0164(13) 0.0203(14) 0.0301(13) -0.0064(10) -0.0005(10) -0.0025(11)
C117 0.0203(13) 0.0268(14) 0.0251(12) -0.0054(10) -0.0025(11) -0.0063(11)
C118 0.0241(16) 0.0326(17) 0.0471(18) -0.0013(14) 0.0116(14) -0.0047(14)
C119 0.0334(19) 0.047(2) 0.079(2) -0.0325(19) 0.0209(17) -0.0275(17)
C120 0.0196(15) 0.077(3) 0.058(2) -0.0450(19) 0.0036(14) -0.0171(16)
C121 0.0155(13) 0.058(2) 0.0341(15) -0.0245(14) -0.0067(12) -0.0017(14)
C122 0.0180(14) 0.081(3) 0.0384(17) -0.0354(17) -0.0070(13) -0.0090(16)
C123 0.0212(14) 0.054(2) 0.0497(18) -0.0382(16) 0.0073(13) -0.0171(14)
C124 0.033(2) 0.053(3) 0.098(3) -0.048(2) 0.017(2) -0.0233(19)
C125 0.0170(13) 0.0300(15) 0.0239(13) -0.0129(11) -0.0013(10) -0.0035(12)
C126 0.0265(14) 0.0191(13) 0.0223(12) -0.0033(10) -0.0068(11) -0.0115(11)
C127 0.047(2) 0.0306(16) 0.0270(14) -0.0029(12) -0.0178(13) -0.0186(15)
C128 0.0279(15) 0.0253(14) 0.0200(12) -0.0058(10) -0.0108(11) -0.0051(12)
C129 0.0278(15) 0.0197(13) 0.0149(11) 0.0001(9) -0.0090(10) -0.0066(12)
C130 0.0166(12) 0.0175(12) 0.0220(12) -0.0058(10) -0.0008(10) -0.0031(10)
C131 0.0197(13) 0.0226(13) 0.0196(12) -0.0017(10) -0.0032(10) -0.0058(11)
C132 0.0202(13) 0.0170(13) 0.0250(12) -0.0010(10) -0.0053(10) -0.0060(10)
C133 0.0206(13) 0.0135(12) 0.0228(12) -0.0030(9) -0.0052(10) -0.0053(10)
C21 0.0119(11) 0.0112(11) 0.0215(11) -0.0047(9) -0.0031(9) 0.0004(9)
C22 0.0192(12) 0.0163(12) 0.0202(12) -0.0036(9) -0.0033(10) -0.0056(10)
```

```
C23 0.0209(13) 0.0208(13) 0.0310(13) -0.0097(10) -0.0054(11) -0.0086(11)
C24 0.0181(13) 0.0147(12) 0.0309(13) -0.0052(10) 0.0016(10) -0.0069(11)
C25 0.0188(13) 0.0137(12) 0.0224(12) 0.0015(9) -0.0036(10) -0.0015(10)
C26 0.0157(12) 0.0154(12) 0.0218(12) -0.0020(9) -0.0033(10) -0.0030(10)
C27 0.0138(11) 0.0143(11) 0.0171(10) 0.0001(9) -0.0040(9) -0.0070(9)
C28 0.0223(13) 0.0178(12) 0.0167(11) -0.0003(9) -0.0050(10) -0.0067(10)
C29 0.0263(14) 0.0210(13) 0.0181(12) -0.0049(10) -0.0017(10) -0.0078(11)
C210 0.0164(13) 0.0174(13) 0.0334(14) -0.0058(10) -0.0043(10) 0.0000(11)
C211 0.0233(14) 0.0210(13) 0.0316(14) -0.0022(10) -0.0139(11) -0.0045(11)
C212 0.0214(13) 0.0192(12) 0.0213(12) -0.0032(10) -0.0082(10) -0.0063(10)
C213 0.0195(12) 0.0122(11) 0.0150(10) 0.0024(8) -0.0070(9) -0.0047(10)
C214 0.0191(12) 0.0149(12) 0.0191(11) 0.0017(9) -0.0075(10) -0.0052(10)
C215 0.0255(14) 0.0193(13) 0.0273(13) 0.0047(10) -0.0153(11) -0.0102(11)
C216 0.0383(16) 0.0192(13) 0.0249(12) -0.0009(10) -0.0171(12) -0.0108(12)
C217 0.0293(14) 0.0210(13) 0.0191(12) -0.0058(10) -0.0057(11) -0.0052(11)
C218 0.0206(13) 0.0185(12) 0.0192(11) -0.0011(9) -0.0049(10) -0.0079(10)
C219 0.0212(12) 0.0130(11) 0.0195(11) -0.0043(9) -0.0092(9) -0.0055(10)
C220 0.0196(13) 0.0193(13) 0.0252(12) -0.0031(10) -0.0088(10) -0.0067(10)
C221 0.0273(15) 0.0185(13) 0.0345(14) -0.0007(10) -0.0192(12) -0.0043(12)
C222 0.0400(16) 0.0163(12) 0.0239(12) 0.0002(10) -0.0196(12) -0.0095(12)
C223 0.0345(15) 0.0175(12) 0.0177(11) -0.0028(9) -0.0086(11) -0.0112(11)
C224 0.0216(13) 0.0165(12) 0.0203(11) -0.0048(9) -0.0073(10) -0.0052(10)
B2 0.0130(12) 0.0156(13) 0.0137(11) -0.0014(9) -0.0039(10) -0.0034(10)
C31 0.079(3) 0.090(4) 0.113(4) 0.047(3) -0.059(3) -0.035(3)
C32 0.231(10) 0.133(6) 0.124(5) 0.047(4) -0.123(7) -0.118(7)
C33 0.322(14) 0.092(5) 0.256(11) 0.078(6) -0.252(12) -0.105(7)
C41 0.048(3) 0.082(4) 0.129(5) 0.030(3) -0.018(3) 0.007(3)
C42 0.053(3) 0.078(4) 0.206(7) 0.012(4) -0.030(4) -0.005(3)
C43 0.289(10) 0.165(7) 0.111(5) 0.042(5) -0.125(6) -0.159(7)
C44 0.121(5) 0.098(4) 0.144(5) -0.045(4) 0.021(4) -0.067(4)
C45 0.210(9) 0.414(15) 0.075(4) 0.076(7) -0.068(5) -0.248(11)
C46 0.168(7) 0.195(8) 0.116(5) -0.092(6) 0.037(5) -0.106(7)

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

# 10. MOLECULAR GEOMETRY

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

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Ti1     O11      2.2180(16)                    .       .                 yes
 Ti1     O12      2.2409(17)                    .       .                 yes
 Ti1     C11        2.419(3)                    .       .                 yes
 Ti1     C12        2.446(3)                    .       .                 yes
 Ti1     C13        2.425(2)                    .       .                 yes
 Ti1     C14        2.431(2)                    .       .                 yes
 Ti1     C15        2.410(2)                    .       .                 yes
 Ti1     C111       2.457(3)                    .       .                 yes
```

Ti1	C112	2.366(3)	.	.	yes
Ti1	C113	2.320(3)	.	.	yes
Ti1	C114	2.369(2)	.	.	yes
Ti1	C115	2.473(3)	.	.	yes
O11	C126	1.469(3)	.	.	yes
O11	C129	1.475(3)	.	.	yes
O12	C130	1.470(3)	.	.	yes
O12	C133	1.480(3)	.	.	yes
C11	C12	1.422(4)	.	.	no
C11	C15	1.432(4)	.	.	no
C11	C16	1.501(4)	.	.	no
C12	C13	1.411(3)	.	.	no
C12	C17	1.502(4)	.	.	no
C13	C14	1.420(4)	.	.	no
C13	C18	1.502(4)	.	.	no
C14	C15	1.414(3)	.	.	no
C14	C19	1.498(4)	.	.	no
C15	C110	1.505(4)	.	.	no
C111	C112	1.400(4)	.	.	no
C111	C115	1.411(3)	.	.	no
C112	C113	1.414(4)	.	.	no
C113	C114	1.409(4)	.	.	no
C114	C115	1.424(4)	.	.	no
C115	C116	1.514(4)	.	.	no
C116	C117	1.547(4)	.	.	no
C116	C123	1.538(4)	.	.	no
C16	H16"	0.9891	.	.	no
C16	H16	0.9185	.	.	no
C16	H16'	0.9491	.	.	no
C117	C118	1.529(4)	.	.	no
C17	H17	1.0111	.	.	no
C17	H17'	1.0254	.	.	no
C17	H17"	0.9691	.	.	no
C117	C125	1.528(4)	.	.	no
C18	H18	0.9447	.	.	no
C18	H18'	0.9521	.	.	no
C118	C119	1.519(6)	.	.	no
C18	H18"	0.9501	.	.	no
C19	H19'	0.9758	.	.	no
C19	H19"	0.9462	.	.	no
C19	H19	0.8765	.	.	no
C119	C120	1.530(6)	.	.	no
C119	C124	1.544(6)	.	.	no
C120	C121	1.524(5)	.	.	no
C121	C122	1.535(4)	.	.	no
C121	C125	1.525(4)	.	.	no
C122	C123	1.533(5)	.	.	no
C123	C124	1.534(5)	.	.	no
C126	C127	1.512(4)	.	.	no
C127	C128	1.515(4)	.	.	no
C128	C129	1.499(4)	.	.	no
C130	C131	1.508(4)	.	.	no
C131	C132	1.523(4)	.	.	no
C132	C133	1.517(4)	.	.	no
C110	H110'	0.9882	.	.	no
C110	H110"	0.9732	.	.	no
C110	H110	0.9905	.	.	no
C111	H111	0.9473	.	.	no
C112	H112	0.9364	.	.	no
C113	H113	0.9648	.	.	no
C114	H114	0.9485	.	.	no

C116	H116	0.9098	.	.	no
C117	H117	0.9766	.	.	no
C118	H118'	0.9417	.	.	no
C118	H118	0.9603	.	.	no
C119	H119	0.9001	.	.	no
C120	H120'	1.0141	.	.	no
C120	H120	0.9507	.	.	no
C121	H121	1.0341	.	.	no
C21	B2	1.645(4)	.	.	yes
C21	C22	1.406(4)	.	.	no
C21	C26	1.407(3)	.	.	no
C122	H122'	0.9942	.	.	no
C22	C23	1.392(4)	.	.	no
C122	H122	0.9987	.	.	no
C123	H123	0.9566	.	.	no
C23	C24	1.385(4)	.	.	no
C124	H124'	0.9513	.	.	no
C24	C25	1.387(4)	.	.	no
C124	H124	0.9906	.	.	no
C25	C26	1.395(4)	.	.	no
C125	H125'	0.9477	.	.	no
C125	H125	0.9931	.	.	no
C126	H126'	1.0365	.	.	no
C126	H126	0.9338	.	.	no
C27	C28	1.406(3)	.	.	no
C127	H127'	0.8820	.	.	no
C127	H127	0.8983	.	.	no
C27	B2	1.644(4)	.	.	yes
C27	C212	1.399(4)	.	.	no
C128	H128'	0.9297	.	.	no
C128	H128	0.9821	.	.	no
C28	C29	1.388(4)	.	.	no
C129	H129	0.9509	.	.	no
C29	C210	1.381(4)	.	.	no
C129	H129'	0.9653	.	.	no
C130	H130'	0.9974	.	.	no
C130	H130	0.9598	.	.	no
C131	H131	0.9901	.	.	no
C131	H131'	0.9703	.	.	no
C132	H132	1.0154	.	.	no
C132	H132'	1.0296	.	.	no
C133	H133	0.9822	.	.	no
C133	H133'	0.9868	.	.	no
C22	H22	1.0295	.	.	no
C23	H23	0.8963	.	.	no
C24	H24	0.9191	.	.	no
C25	H25	0.9881	.	.	no
C26	H26	0.9805	.	.	no
C28	H28	0.9744	.	.	no
C29	H29	0.8947	.	.	no
C210	C211	1.385(4)	.	.	no
C211	C212	1.385(4)	.	.	no
C213	C218	1.404(3)	.	.	no
C213	C214	1.398(4)	.	.	no
C213	B2	1.645(3)	.	.	yes
C214	C215	1.395(3)	.	.	no
C215	C216	1.379(4)	.	.	no
C216	C217	1.379(4)	.	.	no
C217	C218	1.395(4)	.	.	no
C219	C220	1.405(4)	.	.	no
C219	C224	1.398(3)	.	.	no

```
 C219    B2         1.648(3)                    .       .                 yes
 C220    C221       1.393(4)                    .       .                 no
 C221    C222       1.380(4)                    .       .                 no
 C222    C223       1.386(4)                    .       .                 no
 C223    C224       1.390(3)                    .       .                 no
 C31     C33       1.367(12)                    .       .                 no
 C31     C32       1.431(11)                    .       .                 no
 C32     C33       1.122(18)                    .     2_656               no
 C210    H210         0.9563                    .       .                 no
 C211    H211         0.8858                    .       .                 no
 C212    H212         0.9608                    .       .                 no
 C214    H214         0.9518                    .       .                 no
 C215    H215         0.9386                    .       .                 no
 C216    H216         0.9341                    .       .                 no
 C217    H217         0.9551                    .       .                 no
 C218    H218         0.9594                    .       .                 no
 C220    H220         0.9345                    .       .                 no
 C221    H221         0.8874                    .       .                 no
 C222    H222         0.9912                    .       .                 no
 C223    H223         0.9475                    .       .                 no
 C224    H224         0.9530                    .       .                 no
 C31     H31          0.9899                    .       .                 no
 C31     H31'         0.9902                    .       .                 no
 C32     H32          0.9901                    .       .                 no
 C32     H32'         0.9895                    .       .                 no
 C33     H33          0.9903                    .       .                 no
 C33     H33'         0.9895                    .       .                 no
 C41     C43       1.433(10)                    .       .                 no
 C41     C46       1.558(12)                    .       .                 no
 C42     C44       1.365(11)                    .       .                 no
 C42     C45       1.445(13)                    .       .                 no
 C43     C44       1.380(10)                    .       .                 no
 C45     C46       1.442(15)                    .       .                 no
 C41     H41          0.9900                    .       .                 no
 C41     H41'         0.9898                    .       .                 no
 C42     H42          0.9905                    .       .                 no
 C42     H42'         0.9895                    .       .                 no
 C43     H43          0.9898                    .       .                 no
 C43     H43'         0.9900                    .       .                 no
 C44     H44          0.9899                    .       .                 no
 C44     H44'         0.9898                    .       .                 no
 C45     H45          0.9903                    .       .                 no
 C45     H45'         0.9907                    .       .                 no
 C46     H46          0.9905                    .       .                 no
 C46     H46'         0.9903                    .       .                 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
 O11     Ti1     O12        77.78(6)             .       .       .          yes
 O11     Ti1     C11        85.72(7)             .       .       .          yes
 O11     Ti1     C12       113.61(7)             .       .       .          yes
 O11     Ti1     C13       142.25(7)             .       .       .          yes
 O11     Ti1     C14       124.25(7)             .       .       .          yes
 O11     Ti1     C15        91.60(7)             .       .       .          yes
```

O11	Ti1	C111	75.64(7)	.	.	.	yes
O11	Ti1	C112	88.37(7)	.	.	.	yes
O11	Ti1	C113	123.48(8)	.	.	.	yes
O11	Ti1	C114	130.57(8)	.	.	.	yes
O11	Ti1	C115	98.52(7)	.	.	.	yes
O12	Ti1	C11	89.29(7)	.	.	.	yes
O12	Ti1	C12	77.47(7)	.	.	.	yes
O12	Ti1	C13	101.77(8)	.	.	.	yes
O12	Ti1	C14	132.98(8)	.	.	.	yes
O12	Ti1	C15	123.72(8)	.	.	.	yes
O12	Ti1	C111	106.37(7)	.	.	.	yes
O12	Ti1	C112	79.01(8)	.	.	.	yes
O12	Ti1	C113	87.37(8)	.	.	.	yes
O12	Ti1	C114	121.95(7)	.	.	.	yes
O12	Ti1	C115	135.64(7)	.	.	.	yes
C11	Ti1	C12	33.97(8)	.	.	.	yes
C11	Ti1	C13	56.60(8)	.	.	.	yes
C11	Ti1	C14	56.53(8)	.	.	.	yes
C11	Ti1	C15	34.49(9)	.	.	.	yes
C11	Ti1	C111	152.14(9)	.	.	.	yes
C11	Ti1	C112	167.78(9)	.	.	.	yes
C11	Ti1	C113	148.96(9)	.	.	.	yes
C11	Ti1	C114	133.69(8)	.	.	.	yes
C11	Ti1	C115	134.90(8)	.	.	.	yes
C12	Ti1	C13	33.67(8)	.	.	.	yes
C12	Ti1	C14	55.98(9)	.	.	.	yes
C12	Ti1	C15	56.57(9)	.	.	.	yes
C12	Ti1	C111	170.70(8)	.	.	.	yes
C12	Ti1	C112	143.12(9)	.	.	.	yes
C12	Ti1	C113	115.64(9)	.	.	.	yes
C12	Ti1	C114	114.84(8)	.	.	.	yes
C12	Ti1	C115	139.45(8)	.	.	.	yes
C13	Ti1	C14	34.00(9)	.	.	.	yes
C13	Ti1	C15	56.75(8)	.	.	.	yes
C13	Ti1	C111	137.49(8)	.	.	.	yes
C13	Ti1	C112	129.01(8)	.	.	.	yes
C13	Ti1	C113	93.98(9)	.	.	.	yes
C13	Ti1	C114	82.25(9)	.	.	.	yes
C13	Ti1	C115	106.49(8)	.	.	.	yes
C14	Ti1	C15	33.95(7)	.	.	.	yes
C14	Ti1	C111	118.71(9)	.	.	.	yes
C14	Ti1	C112	135.00(8)	.	.	.	yes
C14	Ti1	C113	105.68(8)	.	.	.	yes
C14	Ti1	C114	77.66(8)	.	.	.	yes
C14	Ti1	C115	85.92(8)	.	.	.	yes
C15	Ti1	C111	124.33(9)	.	.	.	yes
C15	Ti1	C112	156.70(10)	.	.	.	yes
C15	Ti1	C113	138.93(8)	.	.	.	yes
C15	Ti1	C114	106.88(8)	.	.	.	yes
C15	Ti1	C115	100.42(8)	.	.	.	yes
C111	Ti1	C112	33.69(9)	.	.	.	yes
C111	Ti1	C113	56.84(9)	.	.	.	yes
C111	Ti1	C114	55.89(9)	.	.	.	yes
C111	Ti1	C115	33.26(8)	.	.	.	yes
C112	Ti1	C113	35.12(9)	.	.	.	yes
C112	Ti1	C114	57.36(8)	.	.	.	yes
C112	Ti1	C115	56.64(8)	.	.	.	yes
C113	Ti1	C114	34.96(9)	.	.	.	yes
C113	Ti1	C115	57.55(9)	.	.	.	yes
C114	Ti1	C115	34.13(9)	.	.	.	yes
Ti1	O11	C126	122.15(13)	.	.	.	yes

Ti1	O11	C129	125.71(13)	.	.	.	yes
C126	O11	C129	106.05(18)	.	.	.	yes
Ti1	O12	C130	126.49(13)	.	.	.	yes
Ti1	O12	C133	124.57(13)	.	.	.	yes
C130	O12	C133	107.87(18)	.	.	.	yes
Ti1	C11	C12	74.05(15)	.	.	.	yes
Ti1	C11	C15	72.41(14)	.	.	.	yes
Ti1	C11	C16	126.60(17)	.	.	.	yes
C12	C11	C15	107.6(2)	.	.	.	no
C12	C11	C16	126.4(2)	.	.	.	no
C15	C11	C16	125.3(2)	.	.	.	no
Ti1	C12	C11	71.98(15)	.	.	.	yes
Ti1	C12	C13	72.35(15)	.	.	.	yes
Ti1	C12	C17	128.23(17)	.	.	.	yes
C11	C12	C13	108.4(2)	.	.	.	no
C11	C12	C17	128.0(2)	.	.	.	no
C13	C12	C17	123.0(2)	.	.	.	no
Ti1	C13	C12	73.98(14)	.	.	.	yes
Ti1	C13	C14	73.23(14)	.	.	.	yes
Ti1	C13	C18	126.04(18)	.	.	.	yes
C12	C13	C14	107.9(2)	.	.	.	no
C12	C13	C18	125.6(3)	.	.	.	no
C14	C13	C18	125.8(2)	.	.	.	no
Ti1	C14	C13	72.77(13)	.	.	.	yes
Ti1	C14	C15	72.21(12)	.	.	.	yes
Ti1	C14	C19	132.8(2)	.	.	.	yes
C13	C14	C15	108.4(2)	.	.	.	no
C13	C14	C19	125.2(2)	.	.	.	no
C15	C14	C19	124.6(2)	.	.	.	no
Ti1	C15	C11	73.10(13)	.	.	.	yes
Ti1	C15	C14	73.84(13)	.	.	.	yes
Ti1	C15	C110	130.7(2)	.	.	.	yes
C11	C15	C14	107.7(2)	.	.	.	no
C11	C15	C110	126.8(2)	.	.	.	no
C14	C15	C110	123.8(2)	.	.	.	no
Ti1	C111	C112	69.60(16)	.	.	.	yes
Ti1	C111	C115	74.03(16)	.	.	.	yes
C112	C111	C115	109.7(2)	.	.	.	no
Ti1	C112	C111	76.71(15)	.	.	.	yes
Ti1	C112	C113	70.68(15)	.	.	.	yes
C111	C112	C113	108.0(2)	.	.	.	no
Ti1	C113	C112	74.21(15)	.	.	.	yes
Ti1	C113	C114	74.40(14)	.	.	.	yes
C112	C113	C114	107.2(2)	.	.	.	no
Ti1	C114	C113	70.64(14)	.	.	.	yes
Ti1	C114	C115	76.97(14)	.	.	.	yes
C113	C114	C115	109.3(2)	.	.	.	no
Ti1	C115	C111	72.72(16)	.	.	.	yes
Ti1	C115	C114	68.90(15)	.	.	.	yes
Ti1	C115	C116	128.09(17)	.	.	.	yes
C111	C115	C114	105.9(2)	.	.	.	no
C111	C115	C116	126.5(2)	.	.	.	no
C114	C115	C116	127.3(2)	.	.	.	no
C115	C116	C117	111.7(2)	.	.	.	no
C115	C116	C123	114.0(2)	.	.	.	no
C117	C116	C123	107.9(2)	.	.	.	no
H16'	C16	H16"	106.72	.	.	.	no
C11	C16	H16'	108.34	.	.	.	no
C11	C16	H16"	109.26	.	.	.	no
C11	C16	H16	112.80	.	.	.	no
H16	C16	H16"	107.13	.	.	.	no

H16	C16	H16'	112.38	.	.	.	no
C118	C117	C125	109.0(2)	.	.	.	no
C116	C117	C125	109.8(2)	.	.	.	no
C116	C117	C118	109.6(2)	.	.	.	no
C12	C17	H17	114.47	.	.	.	no
H17	C17	H17'	108.05	.	.	.	no
H17	C17	H17"	108.23	.	.	.	no
H17'	C17	H17"	104.54	.	.	.	no
C12	C17	H17'	111.38	.	.	.	no
C12	C17	H17"	109.66	.	.	.	no
C13	C18	H18	110.41	.	.	.	no
H18	C18	H18'	101.71	.	.	.	no
C13	C18	H18'	115.14	.	.	.	no
C13	C18	H18"	112.78	.	.	.	no
C117	C118	C119	110.0(3)	.	.	.	no
H18'	C18	H18"	106.16	.	.	.	no
H18	C18	H18"	110.00	.	.	.	no
C118	C119	C124	109.3(3)	.	.	.	no
C118	C119	C120	109.3(3)	.	.	.	no
H19	C19	H19"	101.90	.	.	.	no
C120	C119	C124	109.2(3)	.	.	.	no
H19	C19	H19'	106.02	.	.	.	no
C14	C19	H19	109.65	.	.	.	no
C14	C19	H19'	116.04	.	.	.	no
C14	C19	H19"	116.25	.	.	.	no
H19'	C19	H19"	105.63	.	.	.	no
C119	C120	C121	109.6(3)	.	.	.	no
C120	C121	C122	110.1(3)	.	.	.	no
C120	C121	C125	108.9(2)	.	.	.	no
C122	C121	C125	108.8(3)	.	.	.	no
C121	C122	C123	109.5(2)	.	.	.	no
C116	C123	C122	111.5(3)	.	.	.	no
C116	C123	C124	109.4(3)	.	.	.	no
C122	C123	C124	108.2(3)	.	.	.	no
C119	C124	C123	109.8(3)	.	.	.	no
C117	C125	C121	110.6(2)	.	.	.	no
O11	C126	C127	106.7(2)	.	.	.	yes
C126	C127	C128	104.4(3)	.	.	.	no
C127	C128	C129	101.7(2)	.	.	.	no
O11	C129	C128	103.38(19)	.	.	.	yes
O12	C130	C131	104.93(19)	.	.	.	yes
C130	C131	C132	101.17(19)	.	.	.	no
C131	C132	C133	102.3(2)	.	.	.	no
O12	C133	C132	105.51(19)	.	.	.	yes
C15	C110	H110'	111.55	.	.	.	no
C15	C110	H110"	113.49	.	.	.	no
C15	C110	H110	107.14	.	.	.	no
H110'	C110	H110"	111.01	.	.	.	no
H110'	C110	H110	106.23	.	.	.	no
H110"	C110	H110	106.97	.	.	.	no
Ti1	C111	H111	123.51	.	.	.	no
C112	C111	H111	124.41	.	.	.	no
C115	C111	H111	125.92	.	.	.	no
Ti1	C112	H112	118.86	.	.	.	no
C111	C112	H112	125.15	.	.	.	no
C113	C112	H112	126.87	.	.	.	no
Ti1	C113	H113	118.65	.	.	.	no
C112	C113	H113	127.12	.	.	.	no
C114	C113	H113	125.68	.	.	.	no
Ti1	C114	H114	122.01	.	.	.	no
C113	C114	H114	124.53	.	.	.	no

C115	C114	H114	126.03	.	.	.	no
C115	C116	H116	105.26	.	.	.	no
C117	C116	H116	107.90	.	.	.	no
C123	C116	H116	109.99	.	.	.	no
C116	C117	H117	109.02	.	.	.	no
C118	C117	H117	107.61	.	.	.	no
C125	C117	H117	111.74	.	.	.	no
C117	C118	H118'	107.82	.	.	.	no
C117	C118	H118	107.73	.	.	.	no
C119	C118	H118'	110.40	.	.	.	no
C119	C118	H118	110.51	.	.	.	no
H118'	C118	H118	110.32	.	.	.	no
C118	C119	H119	113.76	.	.	.	no
C120	C119	H119	109.77	.	.	.	no
C124	C119	H119	105.34	.	.	.	no
C119	C120	H120'	107.35	.	.	.	no
C119	C120	H120	112.51	.	.	.	no
C121	C120	H120'	111.00	.	.	.	no
C121	C120	H120	107.51	.	.	.	no
H120'	C120	H120	108.87	.	.	.	no
C120	C121	H121	107.33	.	.	.	no
C122	C121	H121	110.89	.	.	.	no
C125	C121	H121	110.75	.	.	.	no
C26	C21	B2	122.1(2)	.	.	.	yes
C22	C21	C26	115.6(2)	.	.	.	no
C22	C21	B2	121.8(2)	.	.	.	yes
C121	C122	H122	109.36	.	.	.	no
H122'	C122	H122	106.67	.	.	.	no
C123	C122	H122'	108.40	.	.	.	no
C123	C122	H122	111.80	.	.	.	no
C121	C122	H122'	111.15	.	.	.	no
C21	C22	C23	122.2(2)	.	.	.	no
C22	C23	C24	120.7(3)	.	.	.	no
C122	C123	H123	109.81	.	.	.	no
C124	C123	H123	107.79	.	.	.	no
C116	C123	H123	110.01	.	.	.	no
C123	C124	H124'	110.21	.	.	.	no
C123	C124	H124	117.78	.	.	.	no
C119	C124	H124'	102.42	.	.	.	no
C119	C124	H124	105.14	.	.	.	no
C23	C24	C25	118.9(2)	.	.	.	no
H124'	C124	H124	110.31	.	.	.	no
C24	C25	C26	120.2(2)	.	.	.	no
C117	C125	H125	111.27	.	.	.	no
C117	C125	H125'	109.94	.	.	.	no
H125'	C125	H125	104.78	.	.	.	no
C121	C125	H125'	109.49	.	.	.	no
C121	C125	H125	110.64	.	.	.	no
O11	C126	H126	109.09	.	.	.	no
O11	C126	H126'	109.55	.	.	.	no
C127	C126	H126'	110.20	.	.	.	no
C127	C126	H126	115.50	.	.	.	no
H126'	C126	H126	105.73	.	.	.	no
C21	C26	C25	122.5(2)	.	.	.	no
C126	C127	H127'	110.74	.	.	.	no
C128	C127	H127'	112.61	.	.	.	no
C128	C127	H127	106.86	.	.	.	no
C126	C127	H127	108.50	.	.	.	no
C28	C27	C212	115.1(2)	.	.	.	no
C28	C27	B2	123.7(2)	.	.	.	yes
C212	C27	B2	120.69(19)	.	.	.	yes

H127'	C127	H127	113.22	.	.	.	no
C27	C28	C29	122.3(2)	.	.	.	no
C129	C128	H128'	109.75	.	.	.	no
H128'	C128	H128	110.29	.	.	.	no
C127	C128	H128	108.99	.	.	.	no
C129	C128	H128	110.95	.	.	.	no
C127	C128	H128'	114.88	.	.	.	no
O11	C129	H129'	111.09	.	.	.	no
C28	C29	C210	120.7(2)	.	.	.	no
O11	C129	H129	106.89	.	.	.	no
C128	C129	H129'	111.27	.	.	.	no
C128	C129	H129	119.39	.	.	.	no
H129'	C129	H129	104.77	.	.	.	no
C131	C130	H130	116.54	.	.	.	no
H130'	C130	H130	110.57	.	.	.	no
C131	C130	H130'	110.75	.	.	.	no
O12	C130	H130'	107.65	.	.	.	no
O12	C130	H130	105.75	.	.	.	no
C130	C131	H131	111.10	.	.	.	no
C132	C131	H131'	113.82	.	.	.	no
C130	C131	H131'	111.55	.	.	.	no
H131'	C131	H131	106.75	.	.	.	no
C132	C131	H131	112.51	.	.	.	no
C131	C132	H132	111.03	.	.	.	no
C131	C132	H132'	112.08	.	.	.	no
C133	C132	H132	107.63	.	.	.	no
H132'	C132	H132	114.20	.	.	.	no
C133	C132	H132'	108.76	.	.	.	no
C132	C133	H133	114.13	.	.	.	no
H133'	C133	H133	106.93	.	.	.	no
O12	C133	H133'	110.82	.	.	.	no
O12	C133	H133	108.00	.	.	.	no
C132	C133	H133'	111.44	.	.	.	no
C21	C22	H22	117.62	.	.	.	no
C23	C22	H22	120.11	.	.	.	no
C22	C23	H23	120.19	.	.	.	no
C24	C23	H23	119.11	.	.	.	no
C23	C24	H24	121.31	.	.	.	no
C25	C24	H24	119.79	.	.	.	no
C24	C25	H25	122.42	.	.	.	no
C26	C25	H25	117.40	.	.	.	no
C21	C26	H26	118.03	.	.	.	no
C25	C26	H26	119.46	.	.	.	no
C29	C28	H28	116.31	.	.	.	no
C27	C28	H28	121.33	.	.	.	no
C28	C29	H29	119.73	.	.	.	no
C210	C29	H29	119.42	.	.	.	no
C29	C210	C211	118.7(2)	.	.	.	no
C210	C211	C212	120.1(2)	.	.	.	no
C27	C212	C211	123.2(2)	.	.	.	no
C214	C213	C218	115.2(2)	.	.	.	no
C218	C213	B2	122.3(2)	.	.	.	yes
C214	C213	B2	122.2(2)	.	.	.	yes
C213	C214	C215	122.9(2)	.	.	.	no
C214	C215	C216	119.9(3)	.	.	.	no
C215	C216	C217	119.3(2)	.	.	.	no
C216	C217	C218	120.3(2)	.	.	.	no
C213	C218	C217	122.4(3)	.	.	.	no
C220	C219	B2	121.9(2)	.	.	.	yes
C220	C219	C224	115.4(2)	.	.	.	no
C224	C219	B2	122.5(2)	.	.	.	yes

C219	C220	C221	122.4(3)	.	.	.	no
C220	C221	C222	120.4(3)	.	.	.	no
C221	C222	C223	118.7(2)	.	.	.	no
C222	C223	C224	120.5(2)	.	.	.	no
C219	C224	C223	122.5(3)	.	.	.	no
C32	C31	C33	112.2(7)	.	.	.	no
C31	C32	C33	119.2(9)	.	.	2_656	no
C31	C33	C32	99.5(11)	.	.	2_656	no
C29	C210	H210	118.71	.	.	.	no
C211	C210	H210	122.57	.	.	.	no
C212	C211	H211	116.70	.	.	.	no
C210	C211	H211	123.11	.	.	.	no
C211	C212	H212	116.72	.	.	.	no
C27	C212	H212	120.11	.	.	.	no
C213	C214	H214	115.89	.	.	.	no
C215	C214	H214	121.20	.	.	.	no
C216	C215	H215	119.07	.	.	.	no
C214	C215	H215	121.02	.	.	.	no
C217	C216	H216	121.41	.	.	.	no
C215	C216	H216	119.09	.	.	.	no
C218	C217	H217	123.47	.	.	.	no
C216	C217	H217	116.25	.	.	.	no
C213	C218	H218	118.29	.	.	.	no
C217	C218	H218	119.27	.	.	.	no
C219	C220	H220	121.32	.	.	.	no
C221	C220	H220	116.26	.	.	.	no
C220	C221	H221	118.67	.	.	.	no
C222	C221	H221	120.82	.	.	.	no
C223	C222	H222	122.38	.	.	.	no
C221	C222	H222	118.94	.	.	.	no
C222	C223	H223	118.91	.	.	.	no
C224	C223	H223	120.50	.	.	.	no
C219	C224	H224	117.17	.	.	.	no
C223	C224	H224	120.27	.	.	.	no
C33	C31	H31	109.16	.	.	.	no
C32	C31	H31	109.21	.	.	.	no
C32	C31	H31'	109.21	.	.	.	no
H31	C31	H31'	107.88	.	.	.	no
C33	C31	H31'	109.12	.	.	.	no
C31	C32	H32	107.47	.	.	.	no
C31	C32	H32'	107.50	.	.	.	no
C33	C32	H32	107.51	2_656	.	.	no
C33	C32	H32'	107.56	2_656	.	.	no
H32	C32	H32'	107.04	.	.	.	no
C32	C33	H33'	111.88	2_656	.	.	no
C32	C33	H33	111.88	2_656	.	.	no
H33	C33	H33'	109.59	.	.	.	no
C31	C33	H33	111.82	.	.	.	no
C31	C33	H33'	111.89	.	.	.	no
C43	C41	C46	111.6(7)	.	.	.	no
C44	C42	C45	115.2(7)	.	.	.	no
C41	C43	C44	108.2(6)	.	.	.	no
C42	C44	C43	104.7(7)	.	.	.	no
C42	C45	C46	105.7(7)	.	.	.	no
C41	C46	C45	108.7(8)	.	.	.	no
C43	C41	H41'	109.34	.	.	.	no
C46	C41	H41	109.28	.	.	.	no
C43	C41	H41	109.31	.	.	.	no
H41	C41	H41'	107.97	.	.	.	no
C46	C41	H41'	109.30	.	.	.	no
C44	C42	H42	108.43	.	.	.	no

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 C45     C42     H42'         108.47              .       .       .          no
 H42     C42     H42'         107.50              .       .       .          no
 C44     C42     H42'         108.55              .       .       .          no
 C45     C42     H42          108.45              .       .       .          no
 C41     C43     H43          110.06              .       .       .          no
 C44     C43     H43'         110.05              .       .       .          no
 C41     C43     H43'         110.02              .       .       .          no
 C44     C43     H43          110.06              .       .       .          no
 H43     C43     H43'         108.42              .       .       .          no
 C42     C44     H44'         110.88              .       .       .          no
 C43     C44     H44          110.72              .       .       .          no
 C42     C44     H44          110.85              .       .       .          no
 H44     C44     H44'         108.89              .       .       .          no
 C43     C44     H44'         110.75              .       .       .          no
 C42     C45     H45          110.64              .       .       .          no
 H45     C45     H45'         108.67              .       .       .          no
 C46     C45     H45'         110.59              .       .       .          no
 C42     C45     H45'         110.63              .       .       .          no
 C46     C45     H45          110.64              .       .       .          no
 C41     C46     H46'         110.01              .       .       .          no
 H46     C46     H46'         108.28              .       .       .          no
 C45     C46     H46          109.96              .       .       .          no
 C45     C46     H46'         109.93              .       .       .          no
 C41     C46     H46          109.98              .       .       .          no
 C21     B2      C27      102.42(18)              .       .       .          yes
 C21     B2      C213     112.35(18)              .       .       .          yes
 C21     B2      C219       111.9(2)              .       .       .          yes
 C27     B2      C213       111.9(2)              .       .       .          yes
 C27     B2      C219     113.28(18)              .       .       .          yes
 C213    B2      C219     105.29(18)              .       .       .          yes

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
 O12     Ti1     O11     C126     157.58(18)     .       .       .       .   no
 O12     Ti1     O11     C129     -53.78(18)     .       .       .       .   no
 C11     Ti1     O11     C126      67.38(18)     .       .       .       .   no
 C11     Ti1     O11     C129    -143.98(19)     .       .       .       .   no
 C12     Ti1     O11     C126      87.27(18)     .       .       .       .   no
 C12     Ti1     O11     C129    -124.09(19)     .       .       .       .   no
 C13     Ti1     O11     C126        64.1(2)     .       .       .       .   no
 C13     Ti1     O11     C129    -147.29(19)     .       .       .       .   no
 C14     Ti1     O11     C126        23.5(2)     .       .       .       .   no
 C14     Ti1     O11     C129     172.08(18)     .       .       .       .   no
 C15     Ti1     O11     C126      33.38(18)     .       .       .       .   no
 C15     Ti1     O11     C129    -177.99(19)     .       .       .       .   no
 C111    Ti1     O11     C126     -91.74(18)     .       .       .       .   no
 C111    Ti1     O11     C129      56.90(19)     .       .       .       .   no
 C112    Ti1     O11     C126    -123.31(18)     .       .       .       .   no
 C112    Ti1     O11     C129      25.32(19)     .       .       .       .   no
 C113    Ti1     O11     C126    -123.94(18)     .       .       .       .   no
 C113    Ti1     O11     C129        24.7(2)     .       .       .       .   no
 C114    Ti1     O11     C126     -80.59(19)     .       .       .       .   no
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C114	Ti1	O11	C129	68.0(2)	.	.	.	no
C115	Ti1	O11	C126	-67.40(18)	.	.	.	no
C115	Ti1	O11	C129	81.23(19)	.	.	.	no
O11	Ti1	O12	C130	-46.69(18)	.	.	.	no
O11	Ti1	O12	C133	146.61(18)	.	.	.	no
C11	Ti1	O12	C130	39.09(19)	.	.	.	no
C11	Ti1	O12	C133	-127.61(18)	.	.	.	no
C12	Ti1	O12	C130	71.21(18)	.	.	.	no
C12	Ti1	O12	C133	-95.49(18)	.	.	.	no
C13	Ti1	O12	C130	94.69(18)	.	.	.	no
C13	Ti1	O12	C133	-72.01(18)	.	.	.	no
C14	Ti1	O12	C130	79.1(2)	.	.	.	no
C14	Ti1	O12	C133	-87.57(19)	.	.	.	no
C15	Ti1	O12	C130	37.0(2)	.	.	.	no
C15	Ti1	O12	C133	-129.72(17)	.	.	.	no
C111	Ti1	O12	C130	-117.53(18)	.	.	.	no
C111	Ti1	O12	C133	75.77(18)	.	.	.	no
C112	Ti1	O12	C130	-137.40(19)	.	.	.	no
C112	Ti1	O12	C133	55.91(18)	.	.	.	no
C113	Ti1	O12	C130	-171.79(19)	.	.	.	no
C113	Ti1	O12	C133	21.51(18)	.	.	.	no
C114	Ti1	O12	C130	-177.16(18)	.	.	.	no
C114	Ti1	O12	C133	16.1(2)	.	.	.	no
C115	Ti1	O12	C130	-136.41(18)	.	.	.	no
C115	Ti1	O12	C133	56.9(2)	.	.	.	no
O11	Ti1	C11	C12	146.09(14)	.	.	.	no
O11	Ti1	C11	C15	-99.11(14)	.	.	.	no
O11	Ti1	C11	C16	22.2(2)	.	.	.	no
O12	Ti1	C11	C12	68.30(14)	.	.	.	no
O12	Ti1	C11	C15	-176.90(14)	.	.	.	no
O12	Ti1	C11	C16	-55.6(2)	.	.	.	no
C12	Ti1	C11	C15	114.80(19)	.	.	.	no
C12	Ti1	C11	C16	-123.9(3)	.	.	.	no
C13	Ti1	C11	C12	-36.34(13)	.	.	.	no
C13	Ti1	C11	C15	78.47(15)	.	.	.	no
C13	Ti1	C11	C16	-160.2(3)	.	.	.	no
C14	Ti1	C11	C12	-77.35(15)	.	.	.	no
C14	Ti1	C11	C15	37.45(13)	.	.	.	no
C14	Ti1	C11	C16	158.8(3)	.	.	.	no
C15	Ti1	C11	C12	-114.80(19)	.	.	.	no
C15	Ti1	C11	C16	121.4(3)	.	.	.	no
C111	Ti1	C11	C12	-166.28(16)	.	.	.	no
C111	Ti1	C11	C15	-51.5(2)	.	.	.	no
C111	Ti1	C11	C16	69.9(3)	.	.	.	no
C113	Ti1	C11	C12	-15.4(2)	.	.	.	no
C113	Ti1	C11	C15	99.4(2)	.	.	.	no
C113	Ti1	C11	C16	-139.3(2)	.	.	.	no
C114	Ti1	C11	C12	-67.77(18)	.	.	.	no
C114	Ti1	C11	C15	47.03(19)	.	.	.	no
C114	Ti1	C11	C16	168.4(2)	.	.	.	no
C115	Ti1	C11	C12	-116.15(15)	.	.	.	no
C115	Ti1	C11	C15	-1.35(19)	.	.	.	no
C115	Ti1	C11	C16	120.0(2)	.	.	.	no
O11	Ti1	C12	C11	-37.38(15)	.	.	.	no
O11	Ti1	C12	C13	-154.22(13)	.	.	.	no
O11	Ti1	C12	C17	87.3(2)	.	.	.	no
O12	Ti1	C12	C11	-107.88(14)	.	.	.	no
O12	Ti1	C12	C13	135.29(15)	.	.	.	no
O12	Ti1	C12	C17	16.8(2)	.	.	.	no
C11	Ti1	C12	C13	-116.8(2)	.	.	.	no
C11	Ti1	C12	C17	124.7(3)	.	.	.	no

C13	Ti1	C12	C11	116.8(2)	.	.	.	no
C13	Ti1	C12	C17	-118.5(3)	.	.	.	no
C14	Ti1	C12	C11	79.11(15)	.	.	.	no
C14	Ti1	C12	C13	-37.73(14)	.	.	.	no
C14	Ti1	C12	C17	-156.2(2)	.	.	.	no
C15	Ti1	C12	C11	38.02(13)	.	.	.	no
C15	Ti1	C12	C13	-78.82(15)	.	.	.	no
C15	Ti1	C12	C17	162.7(2)	.	.	.	no
C112	Ti1	C12	C11	-159.44(15)	.	.	.	no
C112	Ti1	C12	C13	83.73(19)	.	.	.	no
C112	Ti1	C12	C17	-34.8(3)	.	.	.	no
C113	Ti1	C12	C11	171.26(13)	.	.	.	no
C113	Ti1	C12	C13	54.43(16)	.	.	.	no
C113	Ti1	C12	C17	-64.1(2)	.	.	.	no
C114	Ti1	C12	C11	132.48(14)	.	.	.	no
C114	Ti1	C12	C13	15.65(17)	.	.	.	no
C114	Ti1	C12	C17	-102.9(2)	.	.	.	no
C115	Ti1	C12	C11	102.02(16)	.	.	.	no
C115	Ti1	C12	C13	-14.8(2)	.	.	.	no
C115	Ti1	C12	C17	-133.3(2)	.	.	.	no
O11	Ti1	C13	C12	40.6(2)	.	.	.	no
O11	Ti1	C13	C14	-74.28(18)	.	.	.	no
O11	Ti1	C13	C18	163.3(2)	.	.	.	no
O12	Ti1	C13	C12	-44.55(15)	.	.	.	no
O12	Ti1	C13	C14	-159.46(13)	.	.	.	no
O12	Ti1	C13	C18	78.2(2)	.	.	.	no
C11	Ti1	C13	C12	36.67(14)	.	.	.	no
C11	Ti1	C13	C14	-78.23(15)	.	.	.	no
C11	Ti1	C13	C18	159.4(3)	.	.	.	no
C12	Ti1	C13	C14	-114.9(2)	.	.	.	no
C12	Ti1	C13	C18	122.7(3)	.	.	.	no
C14	Ti1	C13	C12	114.9(2)	.	.	.	no
C14	Ti1	C13	C18	-122.4(3)	.	.	.	no
C15	Ti1	C13	C12	78.22(15)	.	.	.	no
C15	Ti1	C13	C14	-36.68(13)	.	.	.	no
C15	Ti1	C13	C18	-159.1(3)	.	.	.	no
C111	Ti1	C13	C12	-175.35(14)	.	.	.	no
C111	Ti1	C13	C14	69.75(18)	.	.	.	no
C111	Ti1	C13	C18	-52.6(3)	.	.	.	no
C112	Ti1	C13	C12	-129.86(15)	.	.	.	no
C112	Ti1	C13	C14	115.24(15)	.	.	.	no
C112	Ti1	C13	C18	-7.2(3)	.	.	.	no
C113	Ti1	C13	C12	-132.69(15)	.	.	.	no
C113	Ti1	C13	C14	112.41(15)	.	.	.	no
C113	Ti1	C13	C18	-10.0(3)	.	.	.	no
C114	Ti1	C13	C12	-165.70(15)	.	.	.	no
C114	Ti1	C13	C14	79.40(14)	.	.	.	no
C114	Ti1	C13	C18	-43.0(2)	.	.	.	no
C115	Ti1	C13	C12	170.02(14)	.	.	.	no
C115	Ti1	C13	C14	55.12(15)	.	.	.	no
C115	Ti1	C13	C18	-67.3(3)	.	.	.	no
O11	Ti1	C14	C13	134.53(13)	.	.	.	no
O11	Ti1	C14	C15	18.0(2)	.	.	.	no
O11	Ti1	C14	C19	-103.1(2)	.	.	.	no
O12	Ti1	C14	C13	28.01(17)	.	.	.	no
O12	Ti1	C14	C15	-88.54(18)	.	.	.	no
O12	Ti1	C14	C19	150.4(2)	.	.	.	no
C11	Ti1	C14	C13	78.48(16)	.	.	.	no
C11	Ti1	C14	C15	-38.07(16)	.	.	.	no
C11	Ti1	C14	C19	-159.1(3)	.	.	.	no
C12	Ti1	C14	C13	37.35(14)	.	.	.	no

C12	Ti1	C14	C15	-79.20(17)	.	.	.	.	no
C12	Ti1	C14	C19	159.7(3)	.	.	.	.	no
C13	Ti1	C14	C15	-116.5(2)	.	.	.	.	no
C13	Ti1	C14	C19	122.4(3)	.	.	.	.	no
C15	Ti1	C14	C13	116.5(2)	.	.	.	.	no
C15	Ti1	C14	C19	-121.1(3)	.	.	.	.	no
C111	Ti1	C14	C13	-133.71(14)	.	.	.	.	no
C111	Ti1	C14	C15	109.75(17)	.	.	.	.	no
C111	Ti1	C14	C19	-11.3(3)	.	.	.	.	no
C112	Ti1	C14	C13	-96.27(18)	.	.	.	.	no
C112	Ti1	C14	C15	147.19(17)	.	.	.	.	no
C112	Ti1	C14	C19	26.1(3)	.	.	.	.	no
C113	Ti1	C14	C13	-73.31(16)	.	.	.	.	no
C113	Ti1	C14	C15	170.14(16)	.	.	.	.	no
C113	Ti1	C14	C19	49.1(3)	.	.	.	.	no
C114	Ti1	C14	C13	-94.45(15)	.	.	.	.	no
C114	Ti1	C14	C15	149.01(18)	.	.	.	.	no
C114	Ti1	C14	C19	27.9(2)	.	.	.	.	no
C115	Ti1	C14	C13	-127.95(14)	.	.	.	.	no
C115	Ti1	C14	C15	115.51(17)	.	.	.	.	no
C115	Ti1	C14	C19	-5.6(2)	.	.	.	.	no
O11	Ti1	C15	C11	80.07(14)	.	.	.	.	no
O11	Ti1	C15	C14	-165.21(16)	.	.	.	.	no
O11	Ti1	C15	C110	-44.2(2)	.	.	.	.	no
O12	Ti1	C15	C11	3.73(17)	.	.	.	.	no
O12	Ti1	C15	C14	118.44(16)	.	.	.	.	no
O12	Ti1	C15	C110	-120.6(2)	.	.	.	.	no
C11	Ti1	C15	C14	114.7(2)	.	.	.	.	no
C11	Ti1	C15	C110	-124.3(3)	.	.	.	.	no
C12	Ti1	C15	C11	-37.43(14)	.	.	.	.	no
C12	Ti1	C15	C14	77.29(17)	.	.	.	.	no
C12	Ti1	C15	C110	-161.7(2)	.	.	.	.	no
C13	Ti1	C15	C11	-77.99(16)	.	.	.	.	no
C13	Ti1	C15	C14	36.73(16)	.	.	.	.	no
C13	Ti1	C15	C110	157.7(3)	.	.	.	.	no
C14	Ti1	C15	C11	-114.7(2)	.	.	.	.	no
C14	Ti1	C15	C110	121.0(3)	.	.	.	.	no
C111	Ti1	C15	C11	153.73(14)	.	.	.	.	no
C111	Ti1	C15	C14	-91.55(18)	.	.	.	.	no
C111	Ti1	C15	C110	29.4(2)	.	.	.	.	no
C112	Ti1	C15	C11	169.64(19)	.	.	.	.	no
C112	Ti1	C15	C14	-75.6(3)	.	.	.	.	no
C112	Ti1	C15	C110	45.3(3)	.	.	.	.	no
C113	Ti1	C15	C11	-129.25(16)	.	.	.	.	no
C113	Ti1	C15	C14	-14.5(2)	.	.	.	.	no
C113	Ti1	C15	C110	106.5(2)	.	.	.	.	no
C114	Ti1	C15	C11	-146.43(14)	.	.	.	.	no
C114	Ti1	C15	C14	-31.71(18)	.	.	.	.	no
C114	Ti1	C15	C110	89.3(2)	.	.	.	.	no
C115	Ti1	C15	C11	179.03(14)	.	.	.	.	no
C115	Ti1	C15	C14	-66.25(17)	.	.	.	.	no
C115	Ti1	C15	C110	54.7(2)	.	.	.	.	no
O11	Ti1	C111	C112	-109.33(14)	.	.	.	.	no
O11	Ti1	C111	C115	132.00(15)	.	.	.	.	no
O12	Ti1	C111	C112	-36.97(15)	.	.	.	.	no
O12	Ti1	C111	C115	-155.64(14)	.	.	.	.	no
C11	Ti1	C111	C112	-158.84(16)	.	.	.	.	no
C11	Ti1	C111	C115	82.5(2)	.	.	.	.	no
C13	Ti1	C111	C112	92.46(17)	.	.	.	.	no
C13	Ti1	C111	C115	-26.2(2)	.	.	.	.	no
C14	Ti1	C111	C112	129.19(14)	.	.	.	.	no

C14	Ti1	C111	C115	10.52(17)	.	.	.	.	no
C15	Ti1	C111	C112	168.72(13)	.	.	.	.	no
C15	Ti1	C111	C115	50.05(17)	.	.	.	.	no
C112	Ti1	C111	C115	-118.7(2)	.	.	.	.	no
C113	Ti1	C111	C112	38.61(14)	.	.	.	.	no
C113	Ti1	C111	C115	-80.07(15)	.	.	.	.	no
C114	Ti1	C111	C112	80.89(16)	.	.	.	.	no
C114	Ti1	C111	C115	-37.78(14)	.	.	.	.	no
C115	Ti1	C111	C112	118.7(2)	.	.	.	.	no
O11	Ti1	C112	C111	66.14(14)	.	.	.	.	no
O11	Ti1	C112	C113	-179.10(16)	.	.	.	.	no
O12	Ti1	C112	C111	144.00(15)	.	.	.	.	no
O12	Ti1	C112	C113	-101.23(16)	.	.	.	.	no
C12	Ti1	C112	C111	-164.84(14)	.	.	.	.	no
C12	Ti1	C112	C113	-50.1(2)	.	.	.	.	no
C13	Ti1	C112	C111	-119.67(15)	.	.	.	.	no
C13	Ti1	C112	C113	-4.9(2)	.	.	.	.	no
C14	Ti1	C112	C111	-74.01(18)	.	.	.	.	no
C14	Ti1	C112	C113	40.8(2)	.	.	.	.	no
C15	Ti1	C112	C111	-24.1(3)	.	.	.	.	no
C15	Ti1	C112	C113	90.7(3)	.	.	.	.	no
C111	Ti1	C112	C113	114.8(2)	.	.	.	.	no
C113	Ti1	C112	C111	-114.8(2)	.	.	.	.	no
C114	Ti1	C112	C111	-76.12(16)	.	.	.	.	no
C114	Ti1	C112	C113	38.64(15)	.	.	.	.	no
C115	Ti1	C112	C111	-35.17(14)	.	.	.	.	no
C115	Ti1	C112	C113	79.59(16)	.	.	.	.	no
O11	Ti1	C113	C112	1.08(19)	.	.	.	.	no
O11	Ti1	C113	C114	114.50(15)	.	.	.	.	no
O12	Ti1	C113	C112	74.55(16)	.	.	.	.	no
O12	Ti1	C113	C114	-172.03(16)	.	.	.	.	no
C11	Ti1	C113	C112	158.78(17)	.	.	.	.	no
C11	Ti1	C113	C114	-87.8(2)	.	.	.	.	no
C12	Ti1	C113	C112	149.30(15)	.	.	.	.	no
C12	Ti1	C113	C114	-97.27(17)	.	.	.	.	no
C13	Ti1	C113	C112	176.18(16)	.	.	.	.	no
C13	Ti1	C113	C114	-70.40(16)	.	.	.	.	no
C14	Ti1	C113	C112	-151.35(16)	.	.	.	.	no
C14	Ti1	C113	C114	-37.93(18)	.	.	.	.	no
C15	Ti1	C113	C112	-142.99(17)	.	.	.	.	no
C15	Ti1	C113	C114	-29.6(2)	.	.	.	.	no
C111	Ti1	C113	C112	-36.99(15)	.	.	.	.	no
C111	Ti1	C113	C114	76.44(17)	.	.	.	.	no
C112	Ti1	C113	C114	113.4(2)	.	.	.	.	no
C114	Ti1	C113	C112	-113.4(2)	.	.	.	.	no
C115	Ti1	C113	C112	-76.79(17)	.	.	.	.	no
C115	Ti1	C113	C114	36.64(15)	.	.	.	.	no
O11	Ti1	C114	C113	-92.46(17)	.	.	.	.	no
O11	Ti1	C114	C115	23.71(17)	.	.	.	.	no
O12	Ti1	C114	C113	9.40(19)	.	.	.	.	no
O12	Ti1	C114	C115	125.57(13)	.	.	.	.	no
C11	Ti1	C114	C113	134.54(16)	.	.	.	.	no
C11	Ti1	C114	C115	-109.29(16)	.	.	.	.	no
C12	Ti1	C114	C113	99.80(16)	.	.	.	.	no
C12	Ti1	C114	C115	-144.03(13)	.	.	.	.	no
C13	Ti1	C114	C113	108.48(16)	.	.	.	.	no
C13	Ti1	C114	C115	-135.35(14)	.	.	.	.	no
C14	Ti1	C114	C113	142.71(17)	.	.	.	.	no
C14	Ti1	C114	C115	-101.12(14)	.	.	.	.	no
C15	Ti1	C114	C113	160.20(16)	.	.	.	.	no
C15	Ti1	C114	C115	-83.63(15)	.	.	.	.	no

C111	Ti1	C114	C113	-79.38(17)	.	.	.	.	no
C111	Ti1	C114	C115	36.79(13)	.	.	.	.	no
C112	Ti1	C114	C113	-38.82(16)	.	.	.	.	no
C112	Ti1	C114	C115	77.35(15)	.	.	.	.	no
C113	Ti1	C114	C115	116.2(2)	.	.	.	.	no
C115	Ti1	C114	C113	-116.2(2)	.	.	.	.	no
O11	Ti1	C115	C111	-46.72(15)	.	.	.	.	no
O11	Ti1	C115	C114	-162.01(13)	.	.	.	.	no
O11	Ti1	C115	C116	76.5(2)	.	.	.	.	no
O12	Ti1	C115	C111	34.48(19)	.	.	.	.	no
O12	Ti1	C115	C114	-80.81(16)	.	.	.	.	no
O12	Ti1	C115	C116	157.70(18)	.	.	.	.	no
C11	Ti1	C115	C111	-139.16(15)	.	.	.	.	no
C11	Ti1	C115	C114	105.55(16)	.	.	.	.	no
C11	Ti1	C115	C116	-15.9(3)	.	.	.	.	no
C12	Ti1	C115	C111	170.36(14)	.	.	.	.	no
C12	Ti1	C115	C114	55.07(19)	.	.	.	.	no
C12	Ti1	C115	C116	-66.4(3)	.	.	.	.	no
C13	Ti1	C115	C111	161.86(14)	.	.	.	.	no
C13	Ti1	C115	C114	46.57(15)	.	.	.	.	no
C13	Ti1	C115	C116	-74.9(2)	.	.	.	.	no
C14	Ti1	C115	C111	-170.76(15)	.	.	.	.	no
C14	Ti1	C115	C114	73.95(14)	.	.	.	.	no
C14	Ti1	C115	C116	-47.5(2)	.	.	.	.	no
C15	Ti1	C115	C111	-139.94(15)	.	.	.	.	no
C15	Ti1	C115	C114	104.77(14)	.	.	.	.	no
C15	Ti1	C115	C116	-16.7(2)	.	.	.	.	no
C111	Ti1	C115	C114	-115.3(2)	.	.	.	.	no
C111	Ti1	C115	C116	123.2(3)	.	.	.	.	no
C112	Ti1	C115	C111	35.63(14)	.	.	.	.	no
C112	Ti1	C115	C114	-79.66(15)	.	.	.	.	no
C112	Ti1	C115	C116	158.9(2)	.	.	.	.	no
C113	Ti1	C115	C111	77.74(16)	.	.	.	.	no
C113	Ti1	C115	C114	-37.55(14)	.	.	.	.	no
C113	Ti1	C115	C116	-159.0(2)	.	.	.	.	no
C114	Ti1	C115	C111	115.3(2)	.	.	.	.	no
C114	Ti1	C115	C116	-121.5(3)	.	.	.	.	no
C129	O11	C126	C127	13.8(3)	.	.	.	.	no
Ti1	O11	C129	C128	172.06(16)	.	.	.	.	no
Ti1	O11	C126	C127	167.74(18)	.	.	.	.	no
C126	O11	C129	C128	-35.2(3)	.	.	.	.	no
Ti1	O12	C133	C132	162.73(15)	.	.	.	.	no
C130	O12	C133	C132	-6.1(2)	.	.	.	.	no
C133	O12	C130	C131	-20.6(3)	.	.	.	.	no
Ti1	O12	C130	C131	170.92(15)	.	.	.	.	no
Ti1	C11	C12	C13	63.64(17)	.	.	.	.	no
Ti1	C11	C12	C17	-124.9(3)	.	.	.	.	no
C15	C11	C12	Ti1	-65.17(17)	.	.	.	.	no
C12	C11	C15	C110	-165.2(2)	.	.	.	.	no
C16	C11	C15	Ti1	-122.8(2)	.	.	.	.	no
C16	C11	C15	C14	170.9(2)	.	.	.	.	no
C16	C11	C15	C110	5.7(4)	.	.	.	.	no
Ti1	C11	C15	C14	-66.30(16)	.	.	.	.	no
Ti1	C11	C15	C110	128.5(3)	.	.	.	.	no
C15	C11	C12	C13	-1.5(3)	.	.	.	.	no
C15	C11	C12	C17	170.0(2)	.	.	.	.	no
C16	C11	C12	Ti1	124.1(2)	.	.	.	.	no
C16	C11	C12	C13	-172.3(2)	.	.	.	.	no
C16	C11	C12	C17	-0.8(4)	.	.	.	.	no
C12	C11	C15	C14	0.0(3)	.	.	.	.	no
C12	C11	C15	Ti1	66.27(17)	.	.	.	.	no

Ti1	C12	C13	C18	-123.2(2)	.	.	.	.	no
Ti1	C12	C13	C14	65.90(17)	.	.	.	.	no
C11	C12	C13	C14	2.5(3)	.	.	.	.	no
C11	C12	C13	C18	173.4(2)	.	.	.	.	no
C17	C12	C13	Ti1	124.6(2)	.	.	.	.	no
C17	C12	C13	C14	-169.5(2)	.	.	.	.	no
C17	C12	C13	C18	1.4(4)	.	.	.	.	no
C11	C12	C13	Ti1	-63.40(18)	.	.	.	.	no
Ti1	C13	C14	C15	63.87(17)	.	.	.	.	no
C18	C13	C14	C15	-173.4(2)	.	.	.	.	no
C18	C13	C14	C19	-7.9(4)	.	.	.	.	no
C18	C13	C14	Ti1	122.7(3)	.	.	.	.	no
Ti1	C13	C14	C19	-130.6(3)	.	.	.	.	no
C12	C13	C14	Ti1	-66.39(17)	.	.	.	.	no
C12	C13	C14	C15	-2.5(3)	.	.	.	.	no
C12	C13	C14	C19	163.0(2)	.	.	.	.	no
C13	C14	C15	Ti1	-64.24(17)	.	.	.	.	no
C13	C14	C15	C11	1.6(3)	.	.	.	.	no
Ti1	C14	C15	C110	-128.5(3)	.	.	.	.	no
Ti1	C14	C15	C11	65.80(16)	.	.	.	.	no
C19	C14	C15	C11	-164.0(3)	.	.	.	.	no
C19	C14	C15	C110	1.7(4)	.	.	.	.	no
C13	C14	C15	C110	167.3(3)	.	.	.	.	no
C19	C14	C15	Ti1	130.2(3)	.	.	.	.	no
Ti1	C111	C112	H112	116.12	.	.	.	.	no
C115	C111	C112	H112	179.72	.	.	.	.	no
H111	C111	C112	Ti1	-117.34	.	.	.	.	no
H111	C111	C112	C113	178.39	.	.	.	.	no
H111	C111	C112	H112	-1.22	.	.	.	.	no
H111	C111	C115	Ti1	120.12	.	.	.	.	no
H111	C111	C115	C114	-178.60	.	.	.	.	no
H111	C111	C115	C116	-4.88	.	.	.	.	no
Ti1	C112	C113	H113	114.26	.	.	.	.	no
C111	C112	C113	H113	-177.44	.	.	.	.	no
H112	C112	C113	Ti1	-112.11	.	.	.	.	no
H112	C112	C113	C114	-179.78	.	.	.	.	no
H112	C112	C113	H113	2.15	.	.	.	.	no
Ti1	C113	C114	H114	116.12	.	.	.	.	no
C112	C113	C114	H114	-176.34	.	.	.	.	no
H113	C113	C114	Ti1	-114.35	.	.	.	.	no
H113	C113	C114	C115	177.75	.	.	.	.	no
H113	C113	C114	H114	1.76	.	.	.	.	no
H114	C114	C115	Ti1	-120.29	.	.	.	.	no
H114	C114	C115	C111	175.86	.	.	.	.	no
H114	C114	C115	C116	2.21	.	.	.	.	no
Ti1	C115	C116	H116	11.39	.	.	.	.	no
C111	C115	C116	H116	107.74	.	.	.	.	no
C114	C115	C116	H116	-79.86	.	.	.	.	no
C115	C116	C117	H117	-55.31	.	.	.	.	no
C123	C116	C117	H117	178.70	.	.	.	.	no
H116	C116	C117	C118	-57.62	.	.	.	.	no
H116	C116	C117	C125	-177.34	.	.	.	.	no
H116	C116	C117	H117	59.91	.	.	.	.	no
C115	C116	C123	H123	56.14	.	.	.	.	no
C117	C116	C123	H123	-179.23	.	.	.	.	no
H116	C116	C123	C122	176.14	.	.	.	.	no
H116	C116	C123	C124	56.46	.	.	.	.	no
H116	C116	C123	H123	-61.79	.	.	.	.	no
C116	C117	C118	H118'	59.33	.	.	.	.	no
C116	C117	C118	H118	178.38	.	.	.	.	no
C125	C117	C118	H118'	179.56	.	.	.	.	no

C125	C117	C118	H118	-61.39	.	.	.	.	no
H117	C117	C118	C119	-179.51	.	.	.	.	no
H117	C117	C118	H118'	-59.08	.	.	.	.	no
H117	C117	C118	H118	59.98	.	.	.	.	no
C116	C117	C125	H125'	-177.99	.	.	.	.	no
C116	C117	C125	H125	-62.37	.	.	.	.	no
C118	C117	C125	H125'	61.95	.	.	.	.	no
C118	C117	C125	H125	177.57	.	.	.	.	no
H117	C117	C125	C121	-177.87	.	.	.	.	no
H117	C117	C125	H125'	-56.87	.	.	.	.	no
H117	C117	C125	H125	58.75	.	.	.	.	no
C117	C118	C119	H119	176.74	.	.	.	.	no
H118'	C118	C119	C120	-179.02	.	.	.	.	no
H118'	C118	C119	C124	-59.55	.	.	.	.	no
H118'	C118	C119	H119	57.88	.	.	.	.	no
H118	C118	C119	C120	58.66	.	.	.	.	no
H118	C118	C119	C124	178.13	.	.	.	.	no
H118	C118	C119	H119	-64.44	.	.	.	.	no
C118	C119	C120	H120'	-60.06	.	.	.	.	no
C118	C119	C120	H120	-179.82	.	.	.	.	no
C124	C119	C120	H120'	-179.62	.	.	.	.	no
C124	C119	C120	H120	60.62	.	.	.	.	no
H119	C119	C120	C121	-173.96	.	.	.	.	no
H119	C119	C120	H120'	65.37	.	.	.	.	no
H119	C119	C120	H120	-54.38	.	.	.	.	no
C118	C119	C124	H124'	58.02	.	.	.	.	no
C118	C119	C124	H124	173.34	.	.	.	.	no
C120	C119	C124	H124'	177.58	.	.	.	.	no
C120	C119	C124	H124	-67.10	.	.	.	.	no
H119	C119	C124	C123	178.33	.	.	.	.	no
H119	C119	C124	H124'	-64.60	.	.	.	.	no
H119	C119	C124	H124	50.72	.	.	.	.	no
C119	C120	C121	H121	-179.88	.	.	.	.	no
H120'	C120	C121	C122	177.74	.	.	.	.	no
H120'	C120	C121	C125	58.50	.	.	.	.	no
H120'	C120	C121	H121	-61.46	.	.	.	.	no
H120	C120	C121	C122	-63.28	.	.	.	.	no
H120	C120	C121	C125	177.47	.	.	.	.	no
H120	C120	C121	H121	57.51	.	.	.	.	no
C120	C121	C122	H122'	59.24	.	.	.	.	no
C120	C121	C122	H122	176.75	.	.	.	.	no
C125	C121	C122	H122'	178.54	.	.	.	.	no
C125	C121	C122	H122	-63.94	.	.	.	.	no
H121	C121	C122	C123	-179.10	.	.	.	.	no
H121	C121	C122	H122'	-59.40	.	.	.	.	no
H121	C121	C122	H122	58.11	.	.	.	.	no
C120	C121	C125	H125'	-61.63	.	.	.	.	no
C120	C121	C125	H125	-176.62	.	.	.	.	no
C122	C121	C125	H125'	178.33	.	.	.	.	no
C122	C121	C125	H125	63.34	.	.	.	.	no
H121	C121	C125	C117	177.46	.	.	.	.	no
H121	C121	C125	H125'	56.19	.	.	.	.	no
H121	C121	C125	H125	-58.81	.	.	.	.	no
B2	C21	C22	C23	-174.5(2)	.	.	.	.	no
C22	C21	C26	C25	0.9(4)	.	.	.	.	no
B2	C21	C26	C25	173.4(2)	.	.	.	.	no
C22	C21	B2	C27	86.2(3)	.	.	.	.	no
C22	C21	B2	C213	-153.7(2)	.	.	.	.	no
C22	C21	B2	C219	-35.5(3)	.	.	.	.	no
C26	C21	B2	C27	-85.9(2)	.	.	.	.	no
C26	C21	B2	C213	34.3(3)	.	.	.	.	no

C26	C21	B2	C219	152.5(2)	.	.	.	no
C26	C21	C22	C23	-2.0(4)	.	.	.	no
C121	C122	C123	H123	178.18	.	.	.	no
H122'	C122	C123	C116	178.99	.	.	.	no
H122'	C122	C123	C124	-60.61	.	.	.	no
H122'	C122	C123	H123	56.81	.	.	.	no
H122	C122	C123	C116	61.69	.	.	.	no
H122	C122	C123	C124	-177.91	.	.	.	no
C21	C22	C23	C24	1.8(4)	.	.	.	no
H122	C122	C123	H123	-60.49	.	.	.	no
H123	C123	C124	C119	-179.87	.	.	.	no
H123	C123	C124	H124'	68.05	.	.	.	no
C122	C123	C124	H124	59.03	.	.	.	no
C116	C123	C124	H124'	-51.58	.	.	.	no
C116	C123	C124	H124	-179.31	.	.	.	no
H123	C123	C124	H124	-59.68	.	.	.	no
C22	C23	C24	C25	-0.3(4)	.	.	.	no
C122	C123	C124	H124'	-173.24	.	.	.	no
C23	C24	C25	C26	-0.8(4)	.	.	.	no
C24	C25	C26	C21	0.5(4)	.	.	.	no
O11	C126	C127	H127	-101.11	.	.	.	no
O11	C126	C127	H127'	134.06	.	.	.	no
H126'	C126	C127	H127	140.03	.	.	.	no
H126'	C126	C127	C128	-106.27	.	.	.	no
H126'	C126	C127	H127'	15.20	.	.	.	no
H126	C126	C127	H127	20.32	.	.	.	no
H126	C126	C127	C128	134.02	.	.	.	no
H126	C126	C127	H127'	-104.51	.	.	.	no
C212	C27	C28	C29	1.6(4)	.	.	.	no
C126	C127	C128	H128'	-151.89	.	.	.	no
C126	C127	C128	H128	83.78	.	.	.	no
H127'	C127	C128	C129	-153.66	.	.	.	no
H127'	C127	C128	H128'	87.89	.	.	.	no
H127'	C127	C128	H128	-36.44	.	.	.	no
H127	C127	C128	C129	81.42	.	.	.	no
H127	C127	C128	H128'	-37.03	.	.	.	no
H127	C127	C128	H128	-161.36	.	.	.	no
C212	C27	B2	C219	-156.5(2)	.	.	.	no
B2	C27	C28	C29	173.1(2)	.	.	.	no
C28	C27	B2	C21	-88.3(3)	.	.	.	no
C28	C27	B2	C213	151.2(2)	.	.	.	no
C28	C27	B2	C219	32.4(3)	.	.	.	no
C212	C27	B2	C21	82.8(3)	.	.	.	no
C212	C27	B2	C213	-37.7(3)	.	.	.	no
B2	C27	C212	C211	-173.4(2)	.	.	.	no
C28	C27	C212	C211	-1.6(4)	.	.	.	no
C27	C28	C29	C210	-0.3(4)	.	.	.	no
C127	C128	C129	H129'	-77.06	.	.	.	no
H128'	C128	C129	O11	164.30	.	.	.	no
H128	C128	C129	H129	44.92	.	.	.	no
C127	C128	C129	H129	160.72	.	.	.	no
H128	C128	C129	O11	-73.56	.	.	.	no
H128	C128	C129	H129'	167.14	.	.	.	no
H128'	C128	C129	H129'	45.00	.	.	.	no
H128'	C128	C129	H129	-77.22	.	.	.	no
C28	C29	C210	C211	-1.0(4)	.	.	.	no
H130'	C130	C131	C132	-77.33	.	.	.	no
O12	C130	C131	H131	-81.08	.	.	.	no
H130	C130	C131	C132	155.13	.	.	.	no
H130	C130	C131	H131'	-83.49	.	.	.	no
H130	C130	C131	H131	35.49	.	.	.	no

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 O12     C130    C131    H131'       159.94     .       .       .       .   no
 H130'   C130    C131    H131        163.03     .       .       .       .   no
 H130'   C130    C131    H131'        44.05     .       .       .       .   no
 C130    C131    C132    H132       -156.19     .       .       .       .   no
 C130    C131    C132    H132'        74.77     .       .       .       .   no
 H131'   C131    C132    H132         84.04     .       .       .       .   no
 H131    C131    C132    C133         77.04     .       .       .       .   no
 H131    C131    C132    H132'      -166.60     .       .       .       .   no
 H131    C131    C132    H132        -37.56     .       .       .       .   no
 H131'   C131    C132    C133       -161.36     .       .       .       .   no
 H131'   C131    C132    H132'       -45.00     .       .       .       .   no
 H132'   C132    C133    O12         -88.91     .       .       .       .   no
 H132    C132    C133    O12         146.88     .       .       .       .   no
 H132    C132    C133    H133'        26.53     .       .       .       .   no
 H132    C132    C133    H133        -94.72     .       .       .       .   no
 C131    C132    C133    H133        148.22     .       .       .       .   no
 C131    C132    C133    H133'       -90.53     .       .       .       .   no
 H132'   C132    C133    H133         29.49     .       .       .       .   no
 H132'   C132    C133    H133'       150.74     .       .       .       .   no
 C29     C210    C211    C212         1.0(4)    .       .       .       .   no
 C210    C211    C212    C27          0.4(4)    .       .       .       .   no
 C218    C213    B2      C219       -87.9(3)    .       .       .       .   no
 C214    C213    C218    C217         1.5(3)    .       .       .       .   no
 C214    C213    B2      C27        -37.4(3)    .       .       .       .   no
 C214    C213    B2      C219        86.1(3)    .       .       .       .   no
 C218    C213    B2      C27        148.6(2)    .       .       .       .   no
 C218    C213    C214    C215        -1.5(3)    .       .       .       .   no
 B2      C213    C214    C215      -175.9(2)    .       .       .       .   no
 B2      C213    C218    C217       175.9(2)    .       .       .       .   no
 C214    C213    B2      C21       -151.9(2)    .       .       .       .   no
 C218    C213    B2      C21         34.1(3)    .       .       .       .   no
 C213    C214    C215    C216         0.5(4)    .       .       .       .   no
 C214    C215    C216    C217         0.7(4)    .       .       .       .   no
 C215    C216    C217    C218        -0.7(4)    .       .       .       .   no
 C216    C217    C218    C213        -0.4(4)    .       .       .       .   no
 C220    C219    C224    C223         1.7(4)    .       .       .       .   no
 B2      C219    C224    C223       177.2(2)    .       .       .       .   no
 B2      C219    C220    C221      -177.1(2)    .       .       .       .   no
 C224    C219    B2      C21        150.4(2)    .       .       .       .   no
 C224    C219    B2      C27         35.3(3)    .       .       .       .   no
 C224    C219    B2      C213       -87.2(3)    .       .       .       .   no
 C220    C219    B2      C21        -34.4(3)    .       .       .       .   no
 C220    C219    B2      C27       -149.5(2)    .       .       .       .   no
 C220    C219    B2      C213        88.0(3)    .       .       .       .   no
 C224    C219    C220    C221        -1.6(4)    .       .       .       .   no
 C219    C220    C221    C222         0.3(4)    .       .       .       .   no
 C220    C221    C222    C223         1.1(4)    .       .       .       .   no
 C221    C222    C223    C224        -1.0(4)    .       .       .       .   no
 C222    C223    C224    C219        -0.5(4)    .       .       .       .   no
 C33     C31     C32     C33        64.4(12)    .       .       .     2_656 no
 C32     C31     C33     C32       -53.0(10)    .       .       .     2_656 no
 C31     C32     C33     C31       -57.9(10)    .       .     2_656   2_656 no
 C46     C41     C43     C44        -59.3(9)    .       .       .       .   no
 C43     C41     C46     C45         51.8(8)    .       .       .       .   no
 C45     C42     C44     C43        -72.5(8)    .       .       .       .   no
 C44     C42     C45     C46         64.6(9)    .       .       .       .   no
 C41     C43     C44     C42         66.1(8)    .       .       .       .   no
 C42     C45     C46     C41        -49.2(9)    .       .       .       .   no

loop_
_geom_contact_atom_site_label_1
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_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 Ti1     H114         2.9818                    .       .                 no
 Ti1     H116         3.4589                    .       .                 no
 O11     O12        2.799(2)                    .       .                 no
 O11     C11        3.158(3)                    .       .                 no
 O11     C15        3.321(3)                    .       .                 no
 O11     C16        3.366(3)                    .       .                 no
 O11     C111       2.873(3)                    .       .                 no
 O11     C112       3.196(3)                    .       .                 no
 O11     C130       3.095(3)                    .       .                 no
 O12     C112       2.932(3)                    .       .                 no
 O12     C113       3.151(3)                    .       .                 no
 O12     C129       3.149(3)                    .       .                 no
 O12     O11        2.799(2)                    .       .                 no
 O12     C11        3.277(3)                    .       .                 no
 O12     C12        2.937(3)                    .       .                 no
 O12     C17        3.096(3)                    .       .                 no
 O11     H16          2.7862                    .       .                 no
 O11     H111         2.7915                    .       .                 no
 O11     H130         2.4810                    .       .                 no
 O12     H17          2.7291                    .       .                 no
 O12     H112         2.8030                    .       .                 no
 O12     H129         2.5596                    .       .                 no
 C11     O11        3.158(3)                    .       .                 no
 C11     O12        3.277(3)                    .       .                 no
 C11     C13        2.297(3)                    .       .                 no
 C11     C14        2.297(3)                    .       .                 no
 C11     C17        2.628(4)                    .       .                 no
 C11     C33       3.346(13)                    .       .                 no
 C11     C110       2.625(5)                    .       .                 no
 C11     C130       3.511(3)                    .       .                 no
 C12     C33       3.388(11)                    .       .                 no
 C12     C130       3.458(3)                    .       .                 no
 C12     O12        2.937(3)                    .       .                 no
 C12     C14        2.289(4)                    .       .                 no
 C12     C15        2.302(4)                    .       .                 no
 C12     C16        2.609(4)                    .       .                 no
 C12     C18        2.591(4)                    .       .                 no
 C13     C113       3.471(4)                    .       .                 no
 C13     C114       3.153(4)                    .       .                 no
 C13     C15        2.298(3)                    .       .                 no
 C13     C17        2.560(4)                    .       .                 no
 C13     C11        2.297(3)                    .       .                 no
 C13     C19        2.591(4)                    .       .                 no
 C14     C115       3.343(4)                    .       .                 no
 C14     C12        2.289(4)                    .       .                 no
 C14     C114       3.010(3)                    .       .                 no
 C14     C18        2.601(4)                    .       .                 no
 C14     C11        2.297(3)                    .       .                 no
 C14     C110       2.575(4)                    .       .                 no
 C15     O11        3.321(3)                    .       .                 no
 C15     C126       3.428(3)                    .       .                 no
 C15     C12        2.302(4)                    .       .                 no
 C15     C16        2.606(4)                    .       .                 no
 C15     C19        2.578(3)                    .       .                 no
 C15     C13        2.298(3)                    .       .                 no
 C16     C33       3.485(13)                    .       .                 no
```

C16	C126	3.577(4)	.	.	no
C16	C130	3.390(4)	.	.	no
C17	C130	3.301(4)	.	.	no
C17	C133	3.513(4)	.	.	no
C17	C33	3.576(10)	.	.	no
C19	C116	3.435(5)	.	.	no
C22	C220	3.171(3)	.	.	no
C24	C130	3.335(4)	.	2_665	no
C25	C130	3.492(4)	.	2_665	no
C26	C212	3.556(4)	.	.	no
C26	C218	3.178(3)	.	.	no
C28	C224	3.234(3)	.	.	no
C29	C126	3.532(4)	.	1_565	no
C33	C11	3.346(13)	.	.	no
C33	C17	3.576(10)	.	.	no
C33	C12	3.388(11)	.	.	no
C33	C16	3.485(13)	.	.	no
C110	C126	3.291(4)	.	.	no
C11	H130'	3.0931	.	.	no
C11	H33'	2.3916	.	.	no
C111	C116	2.612(4)	.	.	no
C111	C129	3.176(3)	.	.	no
C111	O11	2.873(3)	.	.	no
C111	C113	2.277(4)	.	.	no
C111	C122	3.267(5)	.	.	no
C111	C114	2.263(4)	.	.	no
C112	C129	3.313(3)	.	.	no
C112	C133	3.259(4)	.	.	no
C112	O12	2.932(3)	.	.	no
C112	C115	2.298(3)	.	.	no
C12	H130'	2.9817	.	.	no
C112	O11	3.196(3)	.	.	no
C12	H33'	2.5059	.	.	no
C112	C114	2.272(3)	.	.	no
C113	O12	3.151(3)	.	.	no
C113	C115	2.311(4)	.	.	no
C113	C111	2.277(4)	.	.	no
C113	C133	3.232(4)	.	.	no
C13	H114	3.0164	.	.	no
C113	C13	3.471(4)	.	.	no
C114	C116	2.633(4)	.	.	no
C114	C111	2.263(4)	.	.	no
C114	C125	3.525(4)	.	.	no
C14	H114	2.8833	.	.	no
C114	C19	3.275(4)	.	.	no
C114	C18	3.428(5)	.	.	no
C114	C14	3.010(3)	.	.	no
C114	C112	2.272(3)	.	.	no
C114	C13	3.153(4)	.	.	no
C115	C112	2.298(3)	.	.	no
C115	C19	3.550(4)	.	.	no
C115	C113	2.311(4)	.	.	no
C15	H126'	3.0518	.	.	no
C115	C14	3.343(4)	.	.	no
C116	C120	3.569(5)	.	.	no
C16	H130'	2.8433	.	.	no
C16	H110'	2.8142	.	.	no
C16	H23	3.0804	.	1_545	no
C116	C19	3.435(5)	.	.	no
C16	H33'	2.5932	.	.	no
C16	H17'	2.8490	.	.	no

C16	H126'	2.8590	.	.	no
C17	H130'	2.6021	.	.	no
C17	H33'	2.8322	.	.	no
C17	H16"	2.8384	.	.	no
C17	H18"	2.9615	.	.	no
C18	H17"	3.0298	.	.	no
C118	C122	3.534(4)	.	.	no
C18	H19"	3.0062	.	.	no
C18	H114	2.9927	.	.	no
C19	H116	2.8477	.	.	no
C19	H114	2.8239	.	.	no
C19	H28	2.9780	.	2_566	no
C19	H110	2.9847	.	.	no
C19	H117	2.9793	.	.	no
C19	H18'	2.9109	.	.	no
C120	C116	3.569(5)	.	.	no
C21	H220	2.8236	.	.	no
C21	H218	2.7701	.	.	no
C21	H131'	2.8209	.	2_665	no
C122	C118	3.534(4)	.	.	no
C22	H131'	2.8810	.	2_665	no
C122	C111	3.267(5)	.	.	no
C22	H220	2.8205	.	.	no
C23	H131'	3.0231	.	2_665	no
C23	H24	3.0167	.	2_675	no
C124	C125	3.509(5)	.	.	no
C24	H24	3.0834	.	2_675	no
C24	H128	2.9395	.	1_565	no
C24	H130'	2.9668	.	2_665	no
C25	H130'	2.8389	.	2_665	no
C125	C124	3.509(5)	.	.	no
C25	H211	2.9117	.	2_575	no
C25	H131'	3.0607	.	2_665	no
C125	C114	3.525(4)	.	.	no
C26	H131'	2.8948	.	2_665	no
C26	H127'	3.0648	.	1_565	no
C26	H211	2.9408	.	2_575	no
C126	C16	3.577(4)	.	.	no
C126	C29	3.532(4)	.	1_545	no
C126	C110	3.291(4)	.	.	no
C26	H218	2.7268	.	.	no
C27	H214	2.7546	.	.	no
C27	H224	2.8185	.	.	no
C28	H19	2.9244	.	2_566	no
C28	H224	2.8310	.	.	no
C29	H126	2.9865	.	1_565	no
C29	H19	2.9716	.	2_566	no
C129	C130	3.267(4)	.	.	no
C129	C215	3.583(4)	.	2_565	no
C130	C25	3.492(4)	.	2_665	no
C130	C24	3.335(4)	.	2_665	no
C130	C16	3.390(4)	.	.	no
C130	C129	3.267(4)	.	.	no
C130	C17	3.301(4)	.	.	no
C31	H31'	2.8144	.	2_656	no
C132	C218	3.575(3)	.	.	no
C32	H32'	2.6718	.	2_656	no
C132	C220	3.574(3)	.	.	no
C32	H46	3.0651	.	.	no
C133	C17	3.513(4)	.	.	no
C33	H119	2.8346	.	2_556	no

C41	H42'	2.8460	.	.	no
C42	H41'	3.0316	.	.	no
C45	H43	3.0928	.	.	no
C46	H32	3.0207	.	.	no
C46	H44'	3.0361	.	.	no
C110	H16'	2.9087	.	.	no
C110	H126'	2.7484	.	.	no
C110	H126	2.9816	.	.	no
C110	H19'	2.8495	.	.	no
C111	H122	2.6670	.	.	no
C111	H123	2.8164	.	.	no
C111	H129'	2.6938	.	.	no
C111	H112	2.0847	.	.	no
C112	H111	2.0871	.	.	no
C212	C26	3.556(4)	.	.	no
C112	H129'	2.9880	.	.	no
C212	C214	3.221(3)	.	.	no
C112	H42	2.9235	.	2_566	no
C112	H113	2.1397	.	.	no
C112	H133'	2.8618	.	.	no
C113	H42	3.0432	.	2_566	no
C113	H133	2.9572	.	.	no
C113	H133'	3.0422	.	.	no
C113	H114	2.0977	.	.	no
C113	H112	2.1134	.	.	no
C114	H117	2.7740	.	.	no
C214	C212	3.221(3)	.	.	no
C114	H125	3.0007	.	.	no
C114	H19"	2.9263	.	.	no
C114	H113	2.1219	.	.	no
C215	C129	3.583(4)	.	2_565	no
C115	H122	2.8338	.	.	no
C115	H125	2.7631	.	.	no
C115	H114	2.1255	.	.	no
C115	H111	2.1109	.	.	no
C116	H19'	2.9608	.	.	no
C117	H114	2.9596	.	.	no
C218	C26	3.178(3)	.	.	no
C218	C132	3.575(3)	.	.	no
C119	H33	2.6602	.	2_556	no
C220	C22	3.171(3)	.	.	no
C220	C132	3.574(3)	.	.	no
C121	H125'	3.0556	.	2_466	no
C122	H111	3.0105	.	.	no
C123	H111	2.8016	.	.	no
C224	C28	3.234(3)	.	.	no
C124	H32'	3.0712	.	2_556	no
C124	H33	3.0006	.	2_556	no
C126	H110'	3.0175	.	.	no
C126	H16	3.0093	.	.	no
C127	H211	3.0774	.	2_565	no
C127	H212	2.9940	.	2_565	no
C128	H130	3.0957	.	.	no
C129	H130	2.5584	.	.	no
C129	H112	3.0824	.	.	no
C129	H111	2.8184	.	.	no
C130	H17'	3.0007	.	.	no
C130	H16	2.9571	.	.	no
C130	H129	2.6434	.	.	no
C132	H17	2.9979	.	.	no
C133	H113	2.9057	.	.	no

C133	H17	2.7447	.	.	no
C133	H112	2.9423	.	.	no
C212	H214	2.8154	.	.	no
C212	H128'	3.0446	.	2_565	no
C213	H26	2.7532	.	.	no
C213	H212	2.7700	.	.	no
C213	H133'	3.0593	.	.	no
C214	H133'	2.9432	.	.	no
C214	H212	2.8331	.	.	no
C215	H133'	3.0223	.	.	no
C215	H112	2.8601	.	.	no
C215	H129'	2.7858	.	2_565	no
C217	H132	2.9288	.	.	no
C217	H131	3.0784	.	.	no
C218	H132	2.6845	.	.	no
C218	H26	2.6924	.	.	no
C219	H28	2.8749	.	.	no
C219	H22	2.7246	.	.	no
C220	H22	2.6772	.	.	no
C221	H133	3.0064	.	.	no
C222	H133	2.8622	.	.	no
C222	H18"	2.8543	.	.	no
C222	H117	3.0356	.	2_566	no
C223	H18"	2.9327	.	.	no
C223	H113	2.8668	.	.	no
C223	H133	2.9115	.	.	no
C223	H19"	3.0191	.	2_566	no
C223	H117	3.0042	.	2_566	no
C224	H113	3.0162	.	.	no
C224	H28	2.8240	.	.	no
H110'	H126'	2.2319	.	.	no
H110'	C16	2.8142	.	.	no
H110'	H16'	2.3481	.	.	no
H110'	C126	3.0175	.	.	no
H110"	H116	2.5609	.	.	no
H110"	H126	2.5683	.	.	no
H118'	H116	2.4458	.	.	no
H118'	H124'	2.3900	.	.	no
H120'	H125'	2.5012	.	.	no
H120'	H118	2.4594	.	.	no
H122'	H120	2.5329	.	.	no
H122'	H124	2.5787	.	.	no
H124'	H116	2.4384	.	.	no
H124'	H118'	2.3900	.	.	no
H125'	H120'	2.5012	.	.	no
H125'	H118	2.4927	.	.	no
H125'	C121	3.0556	.	2_466	no
H125'	H121	2.3435	.	2_466	no
H126'	H16	2.3698	.	.	no
H126'	C15	3.0518	.	.	no
H126'	C110	2.7484	.	.	no
H126'	C16	2.8590	.	.	no
H126'	H110'	2.2319	.	.	no
H127'	C26	3.0648	.	1_545	no
H128'	C212	3.0446	.	2_565	no
H128'	H46'	2.5143	.	1_554	no
H128'	H212	2.5617	.	2_565	no
H129'	C215	2.7858	.	2_565	no
H129'	H111	2.1478	.	.	no
H129'	C112	2.9880	.	.	no
H129'	C111	2.6938	.	.	no

H130'	C11	3.0931	.	.	no
H130'	C25	2.8389	.	2_665	no
H130'	C16	2.8433	.	.	no
H130'	C24	2.9668	.	2_665	no
H130'	C12	2.9817	.	.	no
H130'	H17'	2.1011	.	.	no
H130'	H16"	2.5263	.	.	no
H130'	H17	2.5953	.	.	no
H130'	C17	2.6021	.	.	no
H131'	C21	2.8209	.	2_665	no
H131'	C22	2.8810	.	2_665	no
H131'	C26	2.8948	.	2_665	no
H131'	C23	3.0231	.	2_665	no
H131'	C25	3.0607	.	2_665	no
H132'	H17	2.4068	.	.	no
H133'	C113	3.0422	.	.	no
H133'	C214	2.9432	.	.	no
H133'	C213	3.0593	.	.	no
H133'	C112	2.8618	.	.	no
H133'	C215	3.0223	.	.	no
H133'	H112	2.3488	.	.	no
H16	C126	3.0093	.	.	no
H16	O11	2.7862	.	.	no
H16	H23	2.5937	.	1_545	no
H16	H126'	2.3698	.	.	no
H16	H130	2.5372	.	.	no
H16	C130	2.9571	.	.	no
H16'	H110'	2.3481	.	.	no
H16'	C110	2.9087	.	.	no
H16'	H33'	2.5429	.	.	no
H16"	C17	2.8384	.	.	no
H16"	H33'	2.3771	.	.	no
H16"	H130'	2.5263	.	.	no
H16"	H17'	2.2003	.	.	no
H17	H130'	2.5953	.	.	no
H17	C133	2.7447	.	.	no
H17	O12	2.7291	.	.	no
H17	H133	2.3217	.	.	no
H17	H132'	2.4068	.	.	no
H17	C132	2.9979	.	.	no
H17'	C130	3.0007	.	.	no
H17'	C16	2.8490	.	.	no
H17'	H130'	2.1011	.	.	no
H17'	H16"	2.2003	.	.	no
H17"	H32'	2.5010	.	2_656	no
H17"	H31'	2.3963	.	.	no
H17"	H120	2.3975	.	1_655	no
H17"	C18	3.0298	.	.	no
H18'	H19"	2.4832	.	.	no
H18'	C19	2.9109	.	.	no
H18'	H114	2.4598	.	.	no
H18"	C222	2.8543	.	.	no
H18"	C223	2.9327	.	.	no
H18"	C17	2.9615	.	.	no
H18"	H222	2.4571	.	.	no
H18"	H223	2.5447	.	.	no
H19	C28	2.9244	.	2_566	no
H19	H29	2.5091	.	2_566	no
H19	C29	2.9716	.	2_566	no
H19	H28	2.4066	.	2_566	no
H19'	H116	2.2556	.	.	no

H19'	C110	2.8495	.	.	no
H19'	C116	2.9608	.	.	no
H19"	H18'	2.4832	.	.	no
H19"	C18	3.0062	.	.	no
H19"	C114	2.9263	.	.	no
H19"	H117	2.4175	.	.	no
H19"	H114	2.2598	.	.	no
H19"	C223	3.0191	.	2_566	no
H22	H220	2.5422	.	.	no
H22	C220	2.6772	.	.	no
H22	C219	2.7246	.	.	no
H23	C16	3.0804	.	1_565	no
H23	H16	2.5937	.	1_565	no
H23	H24	2.4009	.	2_675	no
H24	C23	3.0167	.	2_675	no
H24	H24	2.5608	.	2_675	no
H24	H23	2.4009	.	2_675	no
H24	C24	3.0834	.	2_675	no
H26	C213	2.7532	.	.	no
H26	C218	2.6924	.	.	no
H26	H218	2.4342	.	.	no
H28	C219	2.8749	.	.	no
H28	H19	2.4066	.	2_566	no
H28	C224	2.8240	.	.	no
H28	C19	2.9780	.	2_566	no
H29	H19	2.5091	.	2_566	no
H31'	H33	2.3186	.	2_656	no
H31'	H32'	1.8948	.	2_656	no
H31'	H17"	2.3963	.	.	no
H31'	C31	2.8144	.	2_656	no
H32	C46	3.0207	.	.	no
H32	H46	2.1610	.	.	no
H32'	H33	2.3847	.	.	no
H32'	H17"	2.5010	.	2_656	no
H32'	H31'	1.8948	.	2_656	no
H32'	C124	3.0712	.	2_556	no
H32'	H124	2.2733	.	2_556	no
H32'	C32	2.6718	.	2_656	no
H33	C124	3.0006	.	2_556	no
H33	H119	1.8648	.	2_556	no
H33	C119	2.6602	.	2_556	no
H33	H31'	2.3186	.	2_656	no
H33	H32'	2.3847	.	.	no
H33'	C16	2.5932	.	.	no
H33'	C11	2.3916	.	.	no
H33'	C12	2.5059	.	.	no
H33'	H16"	2.3771	.	.	no
H33'	H16'	2.5429	.	.	no
H33'	C17	2.8322	.	.	no
H41'	C42	3.0316	.	.	no
H41'	H44'	2.2484	.	.	no
H42	H125	2.5296	.	2_566	no
H42	C113	3.0432	.	2_566	no
H42	C112	2.9235	.	2_566	no
H42'	H46'	2.3386	.	.	no
H42'	H43	1.9871	.	.	no
H42'	C41	2.8460	.	.	no
H43	H46'	2.5907	.	.	no
H43	C45	3.0928	.	.	no
H43	H42'	1.9871	.	.	no
H44	H122	2.5456	.	2_566	no

H44'	H45'	2.3445	.	.	no
H44'	C46	3.0361	.	.	no
H44'	H41'	2.2484	.	.	no
H45'	H44'	2.3445	.	.	no
H46	C32	3.0651	.	.	no
H46	H32	2.1610	.	.	no
H46'	H43	2.5907	.	.	no
H46'	H42'	2.3386	.	.	no
H46'	H128'	2.5143	.	1_556	no
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H111	C122	3.0105	.	.	no
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H111	H122	2.4268	.	.	no
H111	H129'	2.1478	.	.	no
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H112	C133	2.9423	.	.	no
H113	C133	2.9057	.	.	no
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H113	C223	2.8668	.	.	no
H113	H133	2.4175	.	.	no
H114	C14	2.8833	.	.	no
H114	C13	3.0164	.	.	no
H114	H19"	2.2598	.	.	no
H114	H117	2.3784	.	.	no
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H114	C117	2.9596	.	.	no
H114	C18	2.9927	.	.	no
H114	C19	2.8239	.	.	no
H116	C19	2.8477	.	.	no
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H116	H118'	2.4458	.	.	no
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H117	H19"	2.4175	.	.	no
H117	C223	3.0042	.	2_566	no
H117	H114	2.3784	.	.	no
H117	C19	2.9793	.	.	no
H117	C222	3.0356	.	2_566	no
H118	H125'	2.4927	.	.	no
H118	H120'	2.4594	.	.	no
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H120	H122'	2.5329	.	.	no
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H121	H125'	2.3435	.	2_466	no
H122	H125	2.5596	.	.	no
H122	C111	2.6670	.	.	no
H122	H44	2.5456	.	2_566	no
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H122	H111	2.4268	.	.	no
H123	C111	2.8164	.	.	no
H123	H111	2.3823	.	.	no

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H124	H122'	2.5787	.	.	no
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H133	H17	2.3217	.	.	no
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H214	C212	2.8154	.	.	no
H215	H216	2.5852	.	2_565	no
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C130    H130    O11         0.9600     2.4800   3.095(3)     122.00     .   yes

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 'B'  'B'   0.0013   0.0007
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 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.
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C1 C 0.06608(9) 0.7058(2) 0.08790(11) 0.0226(6) Uani 1 1 d . . .
C2 C 0.04589(9) 0.6280(2) 0.04721(11) 0.0227(6) Uani 1 1 d . . .
H2 H 0.0153 0.6304 0.0142 0.027 Uiso 1 1 calc R . .
C3 C 0.07877(9) 0.5455(2) 0.06380(11) 0.0218(5) Uani 1 1 d . . .
H3 H 0.0740 0.4845 0.0433 0.026 Uiso 1 1 calc R . .
C4 C 0.12028(9) 0.5695(2) 0.11643(11) 0.0214(5) Uani 1 1 d . . .
C5 C 0.11206(9) 0.6681(2) 0.12905(11) 0.0221(5) Uani 1 1 d . . .
H5 H 0.1344 0.7051 0.1611 0.027 Uiso 1 1 calc R . .
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C6 C 0.04067(10) 0.8017(2) 0.09178(12) 0.0243(6) Uani 1 1 d . . .
H6 H 0.0484 0.8538 0.0690 0.029 Uiso 1 1 calc R . .
C7 C -0.01587(10) 0.7912(2) 0.06640(13) 0.0316(7) Uani 1 1 d . . .
H7 H -0.0284 0.7650 0.0261 0.038 Uiso 1 1 calc R . .
C8 C -0.03064(12) 0.7204(3) 0.10290(19) 0.0477(9) Uani 1 1 d . . .
H8A H -0.0164 0.6537 0.1036 0.057 Uiso 1 1 calc R . .
H8B H -0.0668 0.7136 0.0858 0.057 Uiso 1 1 calc R . .
C9 C -0.01228(14) 0.7607(3) 0.16453(18) 0.0491(9) Uani 1 1 d . . .
H9 H -0.0220 0.7141 0.1884 0.059 Uiso 1 1 calc R . .
C10 C 0.04377(14) 0.7688(3) 0.19026(15) 0.0459(9) Uani 1 1 d . . .
H10A H 0.0564 0.7938 0.2304 0.055 Uiso 1 1 calc R . .
H10B H 0.0582 0.7022 0.1911 0.055 Uiso 1 1 calc R . .
C11 C 0.05870(11) 0.8397(3) 0.15406(12) 0.0316(7) Uani 1 1 d . . .
H11 H 0.0953 0.8457 0.1716 0.038 Uiso 1 1 calc R . .
C12 C 0.03614(12) 0.9424(3) 0.15313(15) 0.0399(8) Uani 1 1 d . . .
H12A H 0.0484 0.9688 0.1929 0.048 Uiso 1 1 calc R . .
H12B H 0.0460 0.9892 0.1300 0.048 Uiso 1 1 calc R . .
C13 C -0.01983(12) 0.9342(3) 0.12692(14) 0.0355(7) Uani 1 1 d . . .
H13 H -0.0344 1.0015 0.1262 0.043 Uiso 1 1 calc R . .
C14 C -0.03807(12) 0.8944(3) 0.06572(14) 0.0368(7) Uani 1 1 d . . .
H14A H -0.0286 0.9407 0.0421 0.044 Uiso 1 1 calc R . .
H14B H -0.0743 0.8896 0.0482 0.044 Uiso 1 1 calc R . .
C15 C -0.03531(14) 0.8629(3) 0.16262(17) 0.0461(9) Uani 1 1 d . . .
H15A H -0.0715 0.8568 0.1452 0.055 Uiso 1 1 calc R . .
H15B H -0.0245 0.8891 0.2023 0.055 Uiso 1 1 calc R . .
B1 B 0.16427(11) 0.4988(2) 0.16265(13) 0.0227(6) Uani 1 1 d . . .
F1 F 0.24938(7) 0.62221(15) 0.25252(8) 0.0400(5) Uani 1 1 d . . .
F2 F 0.24704(10) 0.7122(2) 0.34230(10) 0.0666(7) Uani 1 1 d . . .
F3 F 0.16662(12) 0.6966(3) 0.36568(10) 0.0842(10) Uani 1 1 d . . .
F4 F 0.08891(9) 0.5820(2) 0.29640(9) 0.0652(7) Uani 1 1 d . . .
F5 F 0.09041(6) 0.48952(17) 0.20514(8) 0.0424(5) Uani 1 1 d . . .
F6A F 0.1685(2) 0.3573(4) 0.2598(2) 0.0439(14) Uiso 0.50 1 d P A 1
F7A F 0.15082(17) 0.1643(4) 0.2484(2) 0.0449(10) Uiso 0.50 1 d P A 1
F8A F 0.12675(16) 0.0702(4) 0.1460(2) 0.0487(10) Uiso 0.50 1 d P A 1
F9A F 0.12152(14) 0.1773(3) 0.05396(19) 0.0390(9) Uiso 0.50 1 d P A 1
F10A F 0.13737(16) 0.3720(4) 0.06246(18) 0.0312(12) Uiso 0.50 1 d P A 1
F6B F 0.1585(2) 0.3394(4) 0.2474(2) 0.0420(14) Uiso 0.50 1 d P B 2
F7B F 0.1371(2) 0.1473(4) 0.2224(2) 0.0597(13) Uiso 0.50 1 d P B 2
F8B F 0.1172(2) 0.0753(4) 0.1159(3) 0.0637(13) Uiso 0.50 1 d P B 2
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C17 C 0.20862(11) 0.6055(3) 0.26187(13) 0.0329(7) Uani 1 1 d . . .
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C19 C 0.16844(16) 0.6475(3) 0.32124(14) 0.0539(11) Uani 1 1 d . . .
C20 C 0.12902(14) 0.5891(3) 0.28583(14) 0.0460(9) Uani 1 1 d . . .
C21 C 0.13097(11) 0.5415(3) 0.23950(13) 0.0350(7) Uani 1 1 d . . .
C22A C 0.15027(8) 0.37605(12) 0.16126(12) 0.0187(14) Uiso 0.50 1 d PG A 1
C23A C 0.15361(10) 0.3216(2) 0.20898(13) 0.0356(15) Uiso 0.50 1 d PG A 1
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C22B C 0.14960(8) 0.37477(12) 0.15021(12) 0.0312(19) Uiso 0.50 1 d PG B 2
C23B C 0.14849(8) 0.31196(17) 0.19283(13) 0.0273(13) Uiso 0.50 1 d PG B 2
C24B C 0.13844(9) 0.21117(15) 0.18137(18) 0.0317(13) Uiso 0.50 1 d PG B 2
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C25B C 0.12949(10) 0.17320(13) 0.12728(19) 0.0316(13) Uiso 0.50 1 d PG B 2
C26B C 0.13060(9) 0.2360(2) 0.08467(15) 0.0313(13) Uiso 0.50 1 d PG B 2
C27B C 0.14066(9) 0.33679(19) 0.09613(12) 0.0383(17) Uiso 0.50 1 d PG B 2
C28 C 0.21675(10) 0.4979(2) 0.15614(12) 0.0251(6) Uani 1 1 d . A .
C29 C 0.25754(10) 0.4467(2) 0.19586(12) 0.0295(6) Uani 1 1 d . . .
C30 C 0.30131(11) 0.4347(3) 0.19166(14) 0.0377(8) Uani 1 1 d . A .
C31 C 0.30648(11) 0.4745(3) 0.14519(16) 0.0414(8) Uani 1 1 d . . .
C32 C 0.26750(11) 0.5247(3) 0.10392(15) 0.0363(7) Uani 1 1 d . A .
C33 C 0.22459(10) 0.5345(2) 0.11081(12) 0.0269(6) Uani 1 1 d . . .
C34 C 0.05985(10) 0.6435(2) -0.06097(11) 0.0286(6) Uani 1 1 d . . .
C35 C 0.10830(11) 0.6173(2) -0.05225(11) 0.0295(6) Uani 1 1 d . . .
C36 C 0.13658(10) 0.7067(2) -0.03893(12) 0.0280(6) Uani 1 1 d . . .
C37 C 0.10557(10) 0.7870(2) -0.03955(12) 0.0279(6) Uani 1 1 d . . .
C38 C 0.05828(10) 0.7472(2) -0.05217(12) 0.0272(6) Uani 1 1 d . . .
C39 C 0.01654(12) 0.5736(3) -0.08416(14) 0.0402(8) Uani 1 1 d . . .
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H39B H 0.0230 0.5161 -0.0584 0.060 Uiso 1 1 calc R . .
H39C H 0.0113 0.5508 -0.1227 0.060 Uiso 1 1 calc R . .
C40 C 0.12477(14) 0.5161(3) -0.06156(15) 0.0449(9) Uani 1 1 d . . .
H40A H 0.1599 0.5180 -0.0524 0.067 Uiso 1 1 calc R . .
H40B H 0.1062 0.4964 -0.1019 0.067 Uiso 1 1 calc R . .
H40C H 0.1190 0.4678 -0.0364 0.067 Uiso 1 1 calc R . .
C41 C 0.18788(11) 0.7177(3) -0.03400(15) 0.0405(8) Uani 1 1 d . . .
H41A H 0.2016 0.6516 -0.0345 0.061 Uiso 1 1 calc R . .
H41B H 0.2083 0.7514 0.0023 0.061 Uiso 1 1 calc R . .
H41C H 0.1873 0.7571 -0.0665 0.061 Uiso 1 1 calc R . .
C42 C 0.11982(12) 0.8950(3) -0.03396(15) 0.0371(7) Uani 1 1 d . . .
H42A H 0.1548 0.9007 -0.0249 0.056 Uiso 1 1 calc R . .
H42B H 0.1135 0.9253 -0.0029 0.056 Uiso 1 1 calc R . .
H42C H 0.1005 0.9294 -0.0704 0.056 Uiso 1 1 calc R . .
C43 C 0.01312(11) 0.8075(3) -0.06269(14) 0.0360(7) Uani 1 1 d . . .
H43A H -0.0147 0.7625 -0.0706 0.054 Uiso 1 1 calc R . .
H43B H 0.0058 0.8515 -0.0959 0.054 Uiso 1 1 calc R . .
H43C H 0.0188 0.8476 -0.0284 0.054 Uiso 1 1 calc R . .
O1 O 0.17315(7) 0.78943(16) 0.08669(9) 0.0283(4) Uani 1 1 d . . .
C44 C 0.22661(11) 0.7837(3) 0.11597(15) 0.0394(8) Uani 1 1 d . . .
H44A H 0.2397 0.7396 0.0948 0.047 Uiso 1 1 calc R . .
H44B H 0.2375 0.7583 0.1558 0.047 Uiso 1 1 calc R . .
C45 C 0.24337(13) 0.8904(3) 0.11615(19) 0.0479(9) Uani 1 1 d . . .
H45A H 0.2489 0.9040 0.0814 0.058 Uiso 1 1 calc R . .
H45B H 0.2741 0.9035 0.1508 0.058 Uiso 1 1 calc R . .
C46 C 0.20142(12) 0.9544(3) 0.11650(15) 0.0388(8) Uani 1 1 d . . .
H46A H 0.1901 1.0028 0.0843 0.047 Uiso 1 1 calc R . .
H46B H 0.2118 0.9911 0.1534 0.047 Uiso 1 1 calc R . .
C47 C 0.16081(12) 0.8792(3) 0.10926(15) 0.0365(7) Uani 1 1 d . . .
H47A H 0.1599 0.8657 0.1468 0.044 Uiso 1 1 calc R . .
H47B H 0.1284 0.9049 0.0820 0.044 Uiso 1 1 calc R . .
O2 O 0.24391(10) 0.63396(17) 0.5020(3) 0.1094(16) Uiso 0.50 1 d PD C -1
C48 C 0.2169(2) 0.7096(3) 0.5155(5) 0.1094(16) Uiso 0.50 1 d PD C -1
H48A H 0.2248 0.7093 0.5572 0.131 Uiso 0.50 1 calc PR C -1
H48B H 0.1812 0.7000 0.4932 0.131 Uiso 0.50 1 calc PR C -1
C49 C 0.23397(13) 0.80723(17) 0.4981(5) 0.1094(16) Uiso 0.50 1 d PD C -1
H49A H 0.2422 0.8575 0.5291 0.131 Uiso 0.50 1 calc PR C -1
H49B H 0.2078 0.8345 0.4624 0.131 Uiso 0.50 1 calc PR C -1
C50 C 0.2797(4) 0.7808(3) 0.4884(8) 0.1094(16) Uiso 0.50 1 d PD C -1
H50A H 0.3084 0.8201 0.5145 0.131 Uiso 0.50 1 calc PR C -1
H50B H 0.2739 0.7948 0.4480 0.131 Uiso 0.50 1 calc PR C -1
C51 C 0.2887(2) 0.6687(5) 0.5016(7) 0.1094(16) Uiso 0.50 1 d PD C -1
H51A H 0.2954 0.6345 0.4714 0.131 Uiso 0.50 1 calc PR C -1
H51B H 0.3167 0.6578 0.5395 0.131 Uiso 0.50 1 calc PR C -1
O3 O 0.02400(13) 0.15923(18) 0.2558(6) 0.278(8) Uiso 0.50 1 d PD D -1
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C52 C -0.01074(18) 0.2389(3) 0.2358(18) 0.278(8) Uiso 0.50 1 d PD D -1
H52A H -0.0346 0.2349 0.2530 0.334 Uiso 0.50 1 calc PR D -1
H52B H -0.0288 0.2377 0.1932 0.334 Uiso 0.50 1 calc PR D -1
C53 C 0.02096(16) 0.33353(19) 0.2561(17) 0.278(8) Uiso 0.50 1 d PD D -1
H53A H 0.0206 0.3709 0.2226 0.334 Uiso 0.50 1 calc PR D -1
H53B H 0.0082 0.3774 0.2778 0.334 Uiso 0.50 1 calc PR D -1
C54 C 0.0734(5) 0.2990(5) 0.2953(13) 0.278(8) Uiso 0.50 1 d PD D -1
H54A H 0.0853 0.3316 0.3336 0.334 Uiso 0.50 1 calc PR D -1
H54B H 0.0962 0.3157 0.2778 0.334 Uiso 0.50 1 calc PR D -1
C55 C 0.0703(7) 0.1853(8) 0.3013(11) 0.278(8) Uiso 0.50 1 d PD D -1
H55A H 0.0975 0.1512 0.2965 0.334 Uiso 0.50 1 calc PR D -1
H55B H 0.0715 0.1676 0.3394 0.334 Uiso 0.50 1 calc PR D -1

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C2 0.0166(12) 0.0269(16) 0.0243(12) 0.0011(10) 0.0084(10) -0.0008(10)
C3 0.0205(12) 0.0211(16) 0.0253(13) -0.0013(10) 0.0112(10) -0.0014(10)
C4 0.0178(12) 0.0211(16) 0.0262(13) 0.0033(10) 0.0103(10) 0.0001(10)
C5 0.0206(12) 0.0247(16) 0.0215(12) -0.0002(10) 0.0093(10) -0.0002(10)
C6 0.0225(13) 0.0211(16) 0.0295(13) -0.0003(11) 0.0112(11) 0.0022(10)
C7 0.0222(13) 0.0319(19) 0.0357(15) -0.0071(12) 0.0073(11) 0.0067(12)
C8 0.0316(17) 0.034(2) 0.088(3) -0.0057(18) 0.0359(18) -0.0011(14)
C9 0.055(2) 0.046(2) 0.067(2) 0.0181(18) 0.0456(19) 0.0174(17)
C10 0.052(2) 0.056(3) 0.0374(17) 0.0132(16) 0.0268(16) 0.0276(18)
C11 0.0244(13) 0.037(2) 0.0300(14) -0.0070(12) 0.0087(11) 0.0053(12)
C12 0.0363(17) 0.039(2) 0.0420(17) -0.0139(14) 0.0141(14) 0.0024(14)
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C14 0.0310(15) 0.037(2) 0.0373(16) -0.0025(13) 0.0097(13) 0.0134(13)
C15 0.0439(19) 0.049(2) 0.057(2) 0.0047(17) 0.0321(17) 0.0158(16)
B1 0.0214(14) 0.0182(17) 0.0267(14) 0.0011(11) 0.0083(11) 0.0013(11)
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F2 0.0701(16) 0.0619(17) 0.0465(12) -0.0258(11) 0.0040(11) 0.0018(12)
F3 0.099(2) 0.111(3) 0.0407(12) -0.0194(13) 0.0282(13) 0.0345(18)
F4 0.0625(14) 0.103(2) 0.0473(12) 0.0196(12) 0.0400(11) 0.0300(14)
F5 0.0319(9) 0.0564(14) 0.0438(10) 0.0087(9) 0.0209(8) -0.0006(8)
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F14 0.0444(11) 0.0662(16) 0.0727(14) 0.0373(12) 0.0430(11) 0.0244(10)
F15 0.0241(8) 0.0336(11) 0.0340(9) 0.0112(7) 0.0152(7) 0.0103(7)
C16 0.0269(14) 0.0258(17) 0.0278(13) 0.0066(11) 0.0101(11) 0.0076(11)
C17 0.0340(15) 0.0298(19) 0.0299(14) 0.0013(12) 0.0087(12) 0.0080(12)
C18 0.054(2) 0.041(2) 0.0286(15) -0.0063(14) 0.0055(14) 0.0111(16)
C19 0.068(3) 0.063(3) 0.0277(16) -0.0016(16) 0.0173(16) 0.028(2)
C20 0.050(2) 0.059(3) 0.0353(17) 0.0148(16) 0.0250(15) 0.0247(18)
C21 0.0331(16) 0.043(2) 0.0279(14) 0.0095(13) 0.0117(12) 0.0097(13)
C28 0.0228(13) 0.0211(16) 0.0301(14) -0.0022(11) 0.0101(11) -0.0003(10)
C29 0.0277(14) 0.0291(18) 0.0291(14) 0.0046(12) 0.0094(11) 0.0047(12)
C30 0.0220(14) 0.038(2) 0.0448(17) 0.0056(14) 0.0058(12) 0.0098(12)
C31 0.0247(15) 0.045(2) 0.060(2) 0.0125(16) 0.0232(14) 0.0111(14)
C32 0.0312(15) 0.034(2) 0.0510(19) 0.0129(14) 0.0250(14) 0.0060(13)
C33 0.0196(12) 0.0230(17) 0.0349(15) 0.0038(11) 0.0085(11) 0.0045(11)
C34 0.0265(14) 0.0341(19) 0.0221(13) 0.0020(11) 0.0074(11) -0.0038(12)
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C35 0.0338(15) 0.0325(19) 0.0227(13) -0.0004(11) 0.0125(11) 0.0015(12)
C36 0.0262(14) 0.0325(18) 0.0275(13) 0.0063(11) 0.0137(11) 0.0017(11)
C37 0.0236(13) 0.0285(18) 0.0312(14) 0.0052(12) 0.0111(11) -0.0014(11)
C38 0.0222(13) 0.0324(18) 0.0256(13) 0.0062(11) 0.0089(10) 0.0007(11)
C39 0.0404(18) 0.042(2) 0.0339(16) -0.0048(14) 0.0116(14) -0.0150(15)
C40 0.059(2) 0.041(2) 0.0373(17) -0.0081(15) 0.0220(16) 0.0070(16)
C41 0.0287(15) 0.053(2) 0.0454(18) 0.0116(16) 0.0213(14) 0.0063(14)
C42 0.0356(16) 0.0268(19) 0.0448(17) 0.0096(13) 0.0130(13) -0.0024(13)
C43 0.0248(14) 0.047(2) 0.0355(15) 0.0144(14) 0.0117(12) 0.0087(13)
O1 0.0225(9) 0.0257(12) 0.0371(11) -0.0045(8) 0.0131(8) -0.0040(8)
C44 0.0228(14) 0.040(2) 0.0483(18) 0.0017(15) 0.0084(13) -0.0034(13)
C45 0.0312(17) 0.041(2) 0.071(2) -0.0110(18) 0.0207(16) -0.0130(14)
C46 0.0392(17) 0.028(2) 0.0495(19) -0.0088(14) 0.0190(15) -0.0109(13)
C47 0.0372(17) 0.0257(19) 0.0514(18) -0.0135(14) 0.0233(14) -0.0071(13)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C4 B1 1.650(4) . ?
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C13 C14 1.520(4) . ?
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B1 C16 1.647(4) . ?
B1 C28 1.656(4) . ?
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B1 C22B 1.717(4) . ?
F1 C17 1.364(4) . ?
F2 C18 1.346(5) . ?
F3 C19 1.335(4) . ?
F4 C20 1.347(4) . ?
F5 C21 1.356(4) . ?
F6A C23A 1.277(6) . ?
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F8A C25A 1.376(5) . ?
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F8B C25B 1.363(6) . ?
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O1 C47 1.451(4) . ?
O1 C44 1.460(4) . ?
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C35 Ti1 C5 156.54(11) . . ?
C1 Ti1 C5 34.89(9) . . ?
O1 Ti1 C37 80.71(9) . . ?
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C5 Ti1 C37 142.55(11) . . ?
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C2 Ti1 C34 78.04(10) . . ?
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F15 Ti1 C38 134.72(8) . . ?
C2 Ti1 C38 83.65(9) . . ?
C3 Ti1 C38 109.31(9) . . ?
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F15 Ti1 C4 73.45(7) . . ?
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O1 Ti1 C4 C3 169.58(15) . . . . ?
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F4 C20 C21 C16 178.6(3) . . . . ?
C19 C20 C21 C16 0.5(5) . . . . ?
C17 C16 C21 F5 177.2(3) . . . . ?
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C17 C16 C21 C20 -0.2(5) . . . . ?
B1 C16 C21 C20 -171.2(3) . . . . ?
C16 B1 C22A C23A -11.8(3) . . . . ?
C4 B1 C22A C23A -125.0(2) . . . . ?
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C22B B1 C22A C23A 170.15(12) . . . . ?
C16 B1 C22A C27A 173.98(17) . . . . ?
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C28 B1 C22A C27A -66.9(2) . . . . ?
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C4 B1 C22B C23B -123.9(2) . . . . ?
C28 B1 C22B C23B 113.43(19) . . . . ?
C22A B1 C22B C23B -5.25(14) . . . . ?
C16 B1 C22B C27B 175.29(18) . . . . ?
C4 B1 C22B C27B 58.7(2) . . . . ?
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C22A B1 C22B C27B 177.43(6) . . . . ?
C27B C22B C23B F6B 177.1(3) . . . . ?
B1 C22B C23B F6B -0.1(4) . . . . ?
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C4 B1 C28 C33 -12.6(4) . . . . ?
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C22B B1 C28 C33 106.2(3) . . . . ?
C16 B1 C28 C29 59.1(4) . . . . ?
C4 B1 C28 C29 175.0(3) . . . . ?
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B1 C28 C29 F11 -5.2(4) . . . . ?
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F11 C29 C30 C31 179.2(3) . . . . ?
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F13 C31 C32 C33 -179.9(3) . . . . ?
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B1 C28 C33 F15 5.0(5) . . . . ?
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F14 C32 C33 F15 1.5(5) . . . . ?
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#===END of Crystallographic Information File
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