Naked (C5Me5)(2)M cations (M = Sc, Ti, and V) and their fluoroarene complexes

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2005

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# CIF-file generated for  C56H60BF2Ti                  CP351

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_audit_update_record
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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,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
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_publ_contact_author_email           A.Meetsma@fwn.rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

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

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2002-07-11  13:32:45
 Date of submission :  2004-05-14  11:07:45


 Consider this CIF submission for deposition of the 8-th
 X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : CP351)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor          ?
_journal_date_accepted               ?

_journal_date_printers_first         ?
_journal_date_printers_final         ?
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# 3. TITLE AND AUTHOR LIST

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;
_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,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;

#=============================================================================
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# 4. TEXT

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;
_publ_section_abstract
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;

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;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
The structure was solved by Patterson methods and extension of the model was
accomplished by direct methods applied to difference structure factors using
the program DIRDIF. The positional and anisotropic thermal displacement
parameters for the non-hydrogen atoms were refined.
Refinement was complicated by a disorder problem: from the solution it was
clear that the F atoms of the solvated fluorobenzene was disordered over two
positions: in opposite orientation to each other. The s.o.f. of the major
component of the disorder model refined to a value of 0.656(5).
A subsequent difference Fourier synthesis showed the positions of most of
the hydrogen atom positions.
;

# Insert blank lines between references

_publ_section_references
;
 Beurskens, P.T., Beurskens, G., Gelder, R. de   Garc\'ia-Granda, S.
  Gould, R.O.  Isra\"el, & Smits, J.M.M. (1994).
  The DIRDIF94 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.

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   Utrecht modified version October 1994.
   Enraf-Nonius, Delft, The Netherlands.

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

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

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```

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  Groningen University, The Netherlands. (unpublished).

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   Acta Cryst. A24, 351-359.

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  Refinement. University of G\"ottingen, Germany, 1993.

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  University, The Netherlands.

Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
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_publ_section_figure_captions
;
     Fig. 1. Chemical structural diagram (scheme 1) of the title compound

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

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

     Fig. 4. Perspective ORTEP drawing of the title compound.
             Displacement ellipsoids for non-H are represented at the 50%
             probability level.
             The H-atoms are drawn with an arbitrary radius.
;

#==

5. CHEMICAL DATA

_chemical_name_systematic
;
 ?
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety
'C26 H35 F Ti, C24 H20 B, C6 H5 F'
_chemical_formula_structural   ?
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C56 H60 B F2 Ti'
_chemical_formula_weight   829.79
_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'
 F   F   0.0171   0.0103
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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

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

_cell_length_a                         11.992(1)
_cell_length_b                         13.649(2)
_cell_length_c                         14.883(1)
_cell_angle_alpha                      90.95(1)
_cell_angle_beta                      109.499(8)
_cell_angle_gamma                      90.865(9)
_cell_volume                          2295.5(4)
_cell_formula_units_Z                     2
_cell_measurement_temperature       130
_cell_measurement_reflns_used       24
_cell_measurement_theta_min         17.06
_cell_measurement_theta_max         17.97
_cell_special_details
;
 Unit cell parameters (Duisenberg, 1992) and orientation matrix were determined
 from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting.

 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           platelet
_exptl_crystal_colour                'orange'
_exptl_crystal_size_max             1.00
_exptl_crystal_size_mid             0.50
_exptl_crystal_size_min             0.10
_exptl_crystal_size_rad              ?
_exptl_crystal_density_meas         ?
_exptl_crystal_density_diffrn           1.200
_exptl_crystal_density_method       'Not Measured'
_exptl_crystal_F_000                      882
_exptl_absorpt_coefficient_mu            0.231
_exptl_crystal_density_meas_temp     ?
_exptl_absorpt_correction_type       'psi-scan'
# Example: '(North, Phillips & Mathews, 1968)'
_exptl_absorpt_process_details       ?
_exptl_absorpt_correction_T_min     0.79
_exptl_absorpt_correction_T_max     0.95

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# 7. EXPERIMENTAL DATA

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 ?
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_diffrn_ambient_temperature         130(1)
_diffrn_radiation_wavelength          0.71073
_diffrn_radiation_type               'MoK\a'
_diffrn_radiation_source             'fine focus sealed Philips Mo tube '
_diffrn_radiation_monochromator      'perpendicular mounted graphite'
_diffrn_radiation_detector
;
  scintillation NaI crystal with photomultiplier
;
_diffrn_measurement_device_type
;
  Enraf Nonius CAD-4F diffractometer
;
_diffrn_measurement_method           '\w/2\q'
_diffrn_special_details
;

 Crystal into the cold nitrogen stream  of the low-temperature unit
   (Bolhuis, 1971), on an Enraf-Nonius CAD-4F diffractometer.
   Graphite-monochromated Mo K\a radiation,
   \w/2\q scan, \D\w = (0.95 + 0.34 tg \q)\%.
;
_diffrn_detector_area_resol_mean     ?

_diffrn_standards_number             1
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      180
_diffrn_standards_decay_%            0.9

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
  2  -1  5

# number of measured reflections (redundant set)
_diffrn_reflns_number                9916
_diffrn_reflns_av_R_equivalents      0.033
_diffrn_reflns_av_sigmaI/netI        0.025
_diffrn_reflns_limit_h_min           -15
_diffrn_reflns_limit_h_max           0
_diffrn_reflns_limit_k_min           -17
_diffrn_reflns_limit_k_max           17
_diffrn_reflns_limit_l_min           -17
_diffrn_reflns_limit_l_max           18
_diffrn_reflns_theta_min             1.45
_diffrn_reflns_theta_max             27.0
_diffrn_reflns_theta_full            27.0

_diffrn_reflns_reduction_process
;

 Intensity data were corrected for Lorentz and polarization effects,
  scale variation, for absorption and reduced to F~o~^2^
;

# number of unique reflections
_reflns_number_total                 9900
# number of observed reflections (> n sig(I))
_reflns_number_gt                    8148
_reflns_threshold_expression         >2sigma(I)

_computing_data_collection           'CAD4-UNIX software Version 5.1, 1994'
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_computing_cell_refinement          'SET4 (de Boer & Duisenberg, 1984)'
_computing_data_reduction           'HELENA (Spek, 1994)'

_computing_structure_solution
;
 DIRDIF-94 (Beurskens et al., 1994)
;
_computing_structure_refinement      'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 1994)
 PLATON (Spek, 1994)
;
_computing_publication_material
;
 PLATON (Spek, 1990)
;

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

# 8. REFINEMENT DATA

_refine_special_details
;
 Refinement on F^2 for ALL reflections except those
 flagged by the user for potential systematic errors.
 Weighted R-factors wR and all goodnesses 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
 observed criterion of F^2 > 2sigma(F^2) is used only
 for calculating -R-factor-obs 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^)+(0.0459P)^2^+3.13P] where P=(Fo^2^+2Fc^2^)/3'
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_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  ?
_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          9284
_refine_ls_number_parameters      561
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           ?
_refine_ls_R_factor_gt            0.0536
_refine_ls_wR_factor_ref          ?
_refine_ls_wR_factor_gt           0.1407
_refine_ls_goodness_of_fit_ref    1.115
_refine_ls_restrained_S_all       1.115
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.48
_refine_diff_density_min         -0.42
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_refine_diff_density_rms         0.06


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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_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 0.24680(4) 0.25660(3) 0.23216(3) 1.000 0.0205(1) . .
F1 F Uani 0.13809(16) 0.25233(12) 0.08423(11) 1.000 0.0430(5) . .
C1 C Uani 0.1681(2) 0.3876(2) 0.29150(19) 1.000 0.0329(8) . .
C2 C Uani 0.2784(2) 0.37084(19) 0.36094(18) 1.000 0.0290(7) . .
C3 C Uani 0.3678(2) 0.38751(18) 0.31945(18) 1.000 0.0278(7) . .
C4 C Uani 0.3119(3) 0.41642(18) 0.22423(19) 1.000 0.0311(8) . .
C5 C Uani 0.1886(3) 0.41836(18) 0.20753(18) 1.000 0.0322(8) . .
C6 C Uani 0.0495(3) 0.3830(3) 0.3062(3) 1.000 0.0560(13) . .
C7 C Uani 0.2983(3) 0.3555(2) 0.46458(19) 1.000 0.0424(10) . .
C8 C Uani 0.4990(3) 0.3897(2) 0.3701(2) 1.000 0.0430(9) . .
C9 C Uani 0.3747(3) 0.4407(2) 0.1551(2) 1.000 0.0475(10) . .
C10 C Uani 0.0945(3) 0.4555(2) 0.1207(2) 1.000 0.0548(11) . .
C11 C Uani 0.2309(2) 0.11513(18) 0.31388(19) 1.000 0.0312(8) . .
C12 C Uani 0.3527(2) 0.13971(19) 0.34195(19) 1.000 0.0326(8) . .
C13 C Uani 0.3878(2) 0.1342(2) 0.2602(2) 1.000 0.0354(9) . .
C14 C Uani 0.2887(3) 0.10187(19) 0.1825(2) 1.000 0.0355(9) . .
C15 C Uani 0.1920(2) 0.09017(18) 0.21568(19) 1.000 0.0313(8) . .
C16 C Uani 0.1569(3) 0.1046(3) 0.3776(3) 1.000 0.0534(11) . .
C17 C Uani 0.4352(3) 0.1482(3) 0.4431(2) 1.000 0.0583(11) . .
C18 C Uani 0.5123(3) 0.1468(3) 0.2594(3) 1.000 0.0663(16) . .
C19 C Uani 0.2903(4) 0.0796(3) 0.0843(3) 1.000 0.0661(14) . .
C20 C Uani 0.0688(3) 0.0541(2) 0.1580(3) 1.000 0.0583(11) . .
C21 C Uani 0.0838(2) 0.26431(19) -0.01405(17) 1.000 0.0298(7) . .
C22 C Uani -0.0335(2) 0.2405(2) -0.05173(19) 1.000 0.0330(8) . .
C23 C Uani -0.0872(2) 0.2542(2) -0.14808(19) 1.000 0.0356(8) . .
C24 C Uani -0.0215(2) 0.2896(2) -0.20186(19) 1.000 0.0358(9) . .
C25 C Uani 0.0972(2) 0.3121(2) -0.1603(2) 1.000 0.0357(8) . .
C26 C Uani 0.1522(2) 0.3001(2) -0.0637(2) 1.000 0.0343(8) . .
C27 C Uani 0.5845(2) 0.66080(16) 0.19054(16) 1.000 0.0212(6) . .
C28 C Uani 0.5814(2) 0.60655(17) 0.10884(17) 1.000 0.0234(7) . .
C29 C Uani 0.6423(2) 0.51937(18) 0.11363(19) 1.000 0.0282(7) . .
C30 C Uani 0.7090(2) 0.48360(18) 0.20132(19) 1.000 0.0304(8) . .
C31 C Uani 0.7158(2) 0.53594(18) 0.28340(19) 1.000 0.0291(7) . .
C32 C Uani 0.6555(2) 0.62302(17) 0.27743(17) 1.000 0.0246(7) . .
C33 C Uani 0.6254(2) 0.84596(16) 0.22714(17) 1.000 0.0227(6) . .
C34 C Uani 0.6589(2) 0.89618(17) 0.31494(18) 1.000 0.0261(7) . .
C35 C Uani 0.7586(2) 0.95818(19) 0.3473(2) 1.000 0.0317(8) . .
C36 C Uani 0.8293(2) 0.97276(19) 0.2917(2) 1.000 0.0332(8) . .
C37 C Uani 0.7994(2) 0.92341(19) 0.2040(2) 1.000 0.0335(8) . .
C38 C Uani 0.7009(2) 0.86224(18) 0.17380(19) 1.000 0.0279(7) . .
C39 C Uani 0.4365(2) 0.76337(17) 0.26009(16) 1.000 0.0219(6) . .
C40 C Uani 0.3872(2) 0.85070(18) 0.27950(18) 1.000 0.0278(7) . .
C41 C Uani 0.3184(2) 0.8554(2) 0.33781(19) 1.000 0.0329(8) . .
C42 C Uani 0.2940(2) 0.7710(2) 0.37916(18) 1.000 0.0332(8) . .
C43 C Uani 0.3369(2) 0.6833(2) 0.35947(18) 1.000 0.0313(8) . .
C44 C Uani 0.4077(2) 0.68026(18) 0.30203(17) 1.000 0.0256(7) . .
C45 C Uani 0.4262(2) 0.78476(17) 0.08179(16) 1.000 0.0221(6) . .
C46 C Uani 0.3320(2) 0.71809(19) 0.03950(18) 1.000 0.0283(7) . .
```

```
C47 C Uani 0.2540(2) 0.7277(2) −0.05218(19) 1.000 0.0339(8) . .
C48 C Uani 0.2643(3) 0.8070(2) −0.10590(19) 1.000 0.0383(9) . .
C49 C Uani 0.3538(3) 0.8753(2) −0.0666(2) 1.000 0.0369(9) . .
C50 C Uani 0.4331(2) 0.86429(18) 0.02528(18) 1.000 0.0288(7) . .
B B Uani 0.5166(2) 0.76487(18) 0.18959(18) 1.000 0.0203(7) . .
F2 F Uani 0.8772(3) 0.46171(19) 0.5069(2) 0.657(6) 0.0537(10) . .
C51 C Uani 0.9060(3) 0.3697(2) 0.4999(2) 1.000 0.0361(8) . .
C52 C Uani 0.8334(2) 0.3102(2) 0.4288(2) 1.000 0.0340(8) . .
C53 C Uani 0.8599(2) 0.2122(2) 0.4272(2) 1.000 0.0345(8) . .
C54 C Uani 0.9585(3) 0.1780(2) 0.4966(2) 1.000 0.0368(9) . .
C55 C Uani 1.0317(3) 0.2387(2) 0.5668(2) 1.000 0.0367(8) . .
C56 C Uani 1.0058(3) 0.3370(2) 0.5684(2) 1.000 0.0368(9) . .
F21 F Uani 0.9767(6) 0.0861(3) 0.4999(4) 0.343(6) 0.0419(17) . .
H6 H Uiso −0.0098(6) 0.3538(18) 0.2493(8) 1.000 0.0841 . .
H6' H Uiso 0.0262(11) 0.4494(3) 0.3173(19) 1.000 0.0841 . .
H6" H Uiso 0.0553(7) 0.3429(16) 0.3615(12) 1.000 0.0841 . .
H7 H Uiso 0.3791(7) 0.3333(16) 0.4958(4) 1.000 0.0636 . .
H7' H Uiso 0.2418(13) 0.3059(12) 0.47115(19) 1.000 0.0636 . .
H7" H Uiso 0.287(2) 0.4173(5) 0.4945(4) 1.000 0.0636 . .
H8 H Uiso 0.5176(3) 0.3492(13) 0.4268(9) 1.000 0.0646 . .
H8' H Uiso 0.5262(4) 0.4574(3) 0.3894(14) 1.000 0.0646 . .
H8" H Uiso 0.5390(3) 0.3641(15) 0.3273(6) 1.000 0.0646 . .
H9 H Uiso 0.4267(16) 0.3870(8) 0.1521(13) 1.000 0.0713 . .
H9' H Uiso 0.4221(17) 0.5012(10) 0.1763(10) 1.000 0.0713 . .
H9" H Uiso 0.3164(3) 0.4499(17) 0.0917(4) 1.000 0.0713 . .
H10 H Uiso 0.0741(17) 0.5223(8) 0.1337(7) 1.000 0.0823 . .
H10' H Uiso 0.0239(9) 0.4127(11) 0.1052(11) 1.000 0.0823 . .
H10" H Uiso 0.1241(9) 0.4557(18) 0.0668(5) 1.000 0.0823 . .
H16 H Uiso 0.1974(11) 0.1377(16) 0.4391(7) 1.000 0.0804 . .
H16' H Uiso 0.145(2) 0.0349(3) 0.3876(15) 1.000 0.0804 . .
H16" H Uiso 0.0799(9) 0.1344(17) 0.3474(9) 1.000 0.0804 . .
H17 H Uiso 0.3921(7) 0.1727(19) 0.4841(4) 1.000 0.0874 . .
H17' H Uiso 0.5005(13) 0.1938(16) 0.4467(4) 1.000 0.0874 . .
H17" H Uiso 0.4668(19) 0.0837(4) 0.4645(7) 1.000 0.0874 . .
H18 H Uiso 0.5116(4) 0.1838(19) 0.2033(12) 1.000 0.0995 . .
H18' H Uiso 0.5459(10) 0.0822(3) 0.257(2) 1.000 0.0995 . .
H18" H Uiso 0.5605(7) 0.1824(19) 0.3173(10) 1.000 0.0995 . .
H19 H Uiso 0.2098(5) 0.083(2) 0.0386(4) 1.000 0.0990 . .
H19' H Uiso 0.321(3) 0.0137(9) 0.0819(6) 1.000 0.0990 . .
H19" H Uiso 0.342(2) 0.1276(14) 0.0679(8) 1.000 0.0990 . .
H20 H Uiso 0.0576(9) 0.0584(19) 0.0899(3) 1.000 0.0877 . .
H20' H Uiso 0.0105(3) 0.0947(13) 0.1733(14) 1.000 0.0877 . .
H20" H Uiso 0.0582(9) −0.0142(7) 0.1734(15) 1.000 0.0877 . .
H22 H Uiso −0.0764(2) 0.2157(2) −0.01340(19) 1.000 0.0396 . .
H23 H Uiso −0.1691(2) 0.2393(2) −0.17753(19) 1.000 0.0428 . .
H24 H Uiso −0.0587(2) 0.2986(2) −0.26828(19) 1.000 0.0430 . .
H25 H Uiso 0.1413(2) 0.3359(2) −0.1981(2) 1.000 0.0428 . .
H26 H Uiso 0.2337(2) 0.3159(2) −0.0333(2) 1.000 0.0412 . .
H28 H Uiso 0.5364(2) 0.63003(17) 0.04802(17) 1.000 0.0280 . .
H29 H Uiso 0.6379(2) 0.48455(18) 0.05672(19) 1.000 0.0338 . .
H30 H Uiso 0.7496(2) 0.42379(18) 0.20505(19) 1.000 0.0365 . .
H31 H Uiso 0.7617(2) 0.51234(18) 0.34392(19) 1.000 0.0349 . .
H32 H Uiso 0.6627(2) 0.65844(17) 0.33465(17) 1.000 0.0295 . .
H34 H Uiso 0.6117(2) 0.88775(17) 0.35446(18) 1.000 0.0313 . .
H35 H Uiso 0.7779(2) 0.99049(19) 0.4078(2) 1.000 0.0380 . .
H36 H Uiso 0.8967(2) 1.01547(19) 0.3128(2) 1.000 0.0398 . .
H37 H Uiso 0.8470(2) 0.93195(19) 0.1648(2) 1.000 0.0402 . .
H38 H Uiso 0.6830(2) 0.82930(18) 0.11377(19) 1.000 0.0335 . .
H40 H Uiso 0.4018(2) 0.90926(18) 0.25123(18) 1.000 0.0333 . .
H41 H Uiso 0.2879(2) 0.9164(2) 0.34949(19) 1.000 0.0395 . .
H42 H Uiso 0.2484(2) 0.7738(2) 0.42044(18) 1.000 0.0398 . .
H43 H Uiso 0.3181(2) 0.6245(2) 0.38516(18) 1.000 0.0375 . .
H44 H Uiso 0.4378(2) 0.61895(18) 0.29087(17) 1.000 0.0308 . .
H46 H Uiso 0.3214(2) 0.66406(19) 0.07551(18) 1.000 0.0339 . .
H47 H Uiso 0.1931(2) 0.6797(2) −0.07845(19) 1.000 0.0407 . .
H48 H Uiso 0.2106(3) 0.8142(2) −0.16876(19) 1.000 0.0459 . .
```

```
H49 H Uiso 0.3615(3) 0.9304(2) -0.1024(2) 1.000 0.0443 . .
H50 H Uiso 0.4941(2) 0.91245(18) 0.05060(18) 1.000 0.0345 . .
H52 H Uiso 0.7662(2) 0.3357(2) 0.3817(2) 1.000 0.0408 . .
H53 H Uiso 0.8109(2) 0.1690(2) 0.3790(2) 1.000 0.0414 . .
H55 H Uiso 1.0993(3) 0.2134(2) 0.6137(2) 1.000 0.0441 . .
H56 H Uiso 1.0557(3) 0.3808(2) 0.6155(2) 1.000 0.0442 . .
H54 H Uiso 0.984(6) 0.115(3) 0.485(5) 0.657(6) 0.0441 . .
H51 H Uiso 0.910(10) 0.435(3) 0.480(8) 0.343(6) 0.0433 . .

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Ti1 0.0191(2) 0.0223(2) 0.0205(2) 0.0010(2) 0.0073(2) 0.0003(2)
F1 0.0523(10) 0.0410(9) 0.0250(8) -0.0018(7) -0.0015(7) 0.0069(8)
C1 0.0302(13) 0.0377(14) 0.0310(13) -0.0099(11) 0.0107(11) 0.0069(11)
C2 0.0302(13) 0.0317(13) 0.0239(12) -0.0046(10) 0.0077(10) -0.0022(10)
C3 0.0289(13) 0.0249(12) 0.0269(12) -0.0019(10) 0.0060(10) -0.0054(10)
C4 0.0430(15) 0.0198(12) 0.0298(13) -0.0005(10) 0.0114(11) -0.0067(10)
C5 0.0427(15) 0.0219(12) 0.0255(12) -0.0041(10) 0.0026(11) 0.0077(11)
C6 0.0335(16) 0.080(3) 0.057(2) -0.0216(18) 0.0193(15) 0.0110(16)
C7 0.0525(18) 0.0514(18) 0.0240(13) -0.0064(12) 0.0143(13) -0.0047(14)
C8 0.0317(15) 0.0459(17) 0.0465(17) -0.0016(14) 0.0071(13) -0.0115(13)
C9 0.071(2) 0.0369(16) 0.0394(16) 0.0001(13) 0.0259(16) -0.0221(15)
C10 0.073(2) 0.0373(17) 0.0418(18) -0.0020(14) 0.0019(16) 0.0262(16)
C11 0.0378(14) 0.0240(12) 0.0370(14) 0.0034(10) 0.0196(12) -0.0032(10)
C12 0.0355(14) 0.0250(12) 0.0335(14) 0.0085(10) 0.0061(11) 0.0019(10)
C13 0.0298(14) 0.0297(13) 0.0526(17) 0.0141(12) 0.0206(13) 0.0096(11)
C14 0.0530(17) 0.0247(13) 0.0369(15) 0.0055(11) 0.0250(13) 0.0145(12)
C15 0.0364(14) 0.0224(12) 0.0331(14) -0.0014(10) 0.0093(11) -0.0018(10)
C16 0.073(2) 0.0429(18) 0.064(2) 0.0086(16) 0.049(2) -0.0055(16)
C17 0.069(2) 0.0434(18) 0.0440(19) 0.0147(15) -0.0064(17) 0.0010(16)
C18 0.0394(18) 0.055(2) 0.120(4) 0.032(2) 0.045(2) 0.0216(16)
C19 0.112(3) 0.054(2) 0.0436(19) 0.0040(16) 0.039(2) 0.042(2)
C20 0.0474(19) 0.0366(17) 0.073(2) -0.0038(16) -0.0030(17) -0.0131(14)
C21 0.0328(13) 0.0293(13) 0.0212(12) -0.0035(10) 0.0010(10) 0.0071(10)
C22 0.0323(14) 0.0379(14) 0.0299(13) -0.0005(11) 0.0120(11) 0.0002(11)
C23 0.0216(12) 0.0510(17) 0.0302(14) -0.0025(12) 0.0036(10) -0.0024(11)
C24 0.0292(14) 0.0506(17) 0.0264(13) -0.0002(12) 0.0075(11) 0.0027(12)
C25 0.0325(14) 0.0435(16) 0.0350(14) -0.0019(12) 0.0167(12) 0.0006(12)
C26 0.0225(12) 0.0390(15) 0.0388(15) -0.0076(12) 0.0071(11) 0.0006(11)
C27 0.0216(11) 0.0182(10) 0.0263(11) 0.0005(9) 0.0116(9) -0.0033(8)
C28 0.0228(11) 0.0233(11) 0.0247(12) 0.0007(9) 0.0090(9) -0.0014(9)
C29 0.0301(13) 0.0252(12) 0.0316(13) -0.0050(10) 0.0135(11) 0.0014(10)
C30 0.0271(12) 0.0232(12) 0.0417(15) 0.0021(10) 0.0123(11) 0.0054(10)
C31 0.0287(13) 0.0252(12) 0.0318(13) 0.0059(10) 0.0076(10) 0.0028(10)
C32 0.0251(12) 0.0234(11) 0.0261(12) 0.0006(9) 0.0096(10) -0.0004(9)
C33 0.0232(11) 0.0166(10) 0.0313(12) 0.0039(9) 0.0127(10) 0.0023(9)
C34 0.0267(12) 0.0214(11) 0.0300(12) 0.0026(9) 0.0093(10) -0.0008(9)
C35 0.0336(14) 0.0245(12) 0.0335(14) 0.0000(10) 0.0068(11) -0.0029(10)
C36 0.0243(12) 0.0242(12) 0.0468(16) 0.0045(11) 0.0064(11) -0.0057(10)
C37 0.0293(13) 0.0297(13) 0.0455(16) 0.0076(12) 0.0177(12) -0.0013(10)
C38 0.0278(12) 0.0250(12) 0.0350(13) 0.0005(10) 0.0159(11) -0.0004(10)
C39 0.0185(10) 0.0245(11) 0.0212(11) -0.0021(9) 0.0050(9) -0.0029(9)
C40 0.0266(12) 0.0246(12) 0.0345(13) -0.0006(10) 0.0135(10) 0.0006(10)
C41 0.0259(13) 0.0374(14) 0.0368(14) -0.0074(11) 0.0126(11) 0.0028(11)
C42 0.0224(12) 0.0547(17) 0.0231(12) -0.0041(11) 0.0089(10) -0.0025(11)
C43 0.0249(12) 0.0415(15) 0.0271(13) 0.0063(11) 0.0083(10) -0.0048(11)
C44 0.0237(12) 0.0262(12) 0.0272(12) 0.0008(10) 0.0088(10) -0.0014(9)
C45 0.0204(11) 0.0239(11) 0.0242(11) -0.0008(9) 0.0101(9) 0.0044(9)
C46 0.0244(12) 0.0302(13) 0.0302(13) 0.0015(10) 0.0090(10) 0.0026(10)
C47 0.0235(12) 0.0425(15) 0.0329(14) -0.0072(12) 0.0058(11) 0.0036(11)
```

```
C48 0.0362(15) 0.0513(17) 0.0252(13) 0.0008(12) 0.0068(11) 0.0164(13)
C49 0.0453(16) 0.0361(15) 0.0314(14) 0.0091(11) 0.0147(12) 0.0136(12)
C50 0.0336(13) 0.0240(12) 0.0311(13) 0.0034(10) 0.0135(11) 0.0052(10)
B 0.0211(12) 0.0186(12) 0.0224(12) 0.0002(9) 0.0089(10) -0.0009(9)
F2 0.071(2) 0.0264(14) 0.0505(19) 0.0008(12) 0.0023(14) 0.0108(13)
C51 0.0398(15) 0.0289(14) 0.0395(15) 0.0006(12) 0.0132(12) 0.0027(12)
C52 0.0300(13) 0.0361(14) 0.0348(14) 0.0048(11) 0.0092(11) 0.0024(11)
C53 0.0327(14) 0.0337(14) 0.0386(15) -0.0043(11) 0.0145(12) -0.0049(11)
C54 0.0401(16) 0.0309(14) 0.0443(16) 0.0010(12) 0.0205(13) 0.0046(12)
C55 0.0336(14) 0.0424(16) 0.0350(14) 0.0084(12) 0.0119(12) 0.0089(12)
C56 0.0405(16) 0.0367(15) 0.0319(14) -0.0021(11) 0.0107(12) -0.0049(12)
F21 0.047(3) 0.026(3) 0.047(3) 0.000(2) 0.008(2) 0.007(2)

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

# 10. MOLECULAR GEOMETRY

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

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
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 Ti1     F1       2.1512(17)                    .       .                 yes
 Ti1     C1         2.329(3)                    .       .                 yes
 Ti1     C2         2.376(3)                    .       .                 yes
 Ti1     C3         2.361(3)                    .       .                 yes
 Ti1     C4         2.324(3)                    .       .                 yes
 Ti1     C5         2.324(3)                    .       .                 yes
 Ti1     C11        2.338(3)                    .       .                 yes
 Ti1     C12        2.364(3)                    .       .                 yes
 Ti1     C13        2.337(3)                    .       .                 yes
 Ti1     C14        2.342(3)                    .       .                 yes
 Ti1     C15        2.341(3)                    .       .                 yes
 F1      C21        1.402(3)                    .       .                 yes
 F2      C51        1.319(4)                    .       .                 yes
 F21     C54        1.275(5)                    .       .                 yes
 C1      C6         1.510(5)                    .       .                 no
 C1      C5         1.421(4)                    .       .                 no
 C1      C2         1.405(4)                    .       .                 no
 C2      C3         1.422(4)                    .       .                 no
 C2      C7         1.499(4)                    .       .                 no
 C3      C8         1.500(4)                    .       .                 no
 C3      C4         1.416(4)                    .       .                 no
 C4      C9         1.502(5)                    .       .                 no
 C4      C5         1.416(5)                    .       .                 no
 C5      C10        1.505(4)                    .       .                 no
 C11     C15        1.412(4)                    .       .                 no
 C11     C12        1.412(4)                    .       .                 no
 C11     C16        1.507(5)                    .       .                 no
 C12     C17        1.502(4)                    .       .                 no
 C12     C13        1.415(4)                    .       .                 no
 C13     C14        1.412(4)                    .       .                 no
 C13     C18        1.504(5)                    .       .                 no
 C14     C19        1.494(5)                    .       .                 no
 C14     C15        1.412(4)                    .       .                 no
```

C15	C20	1.510(5)	.	.	no
C21	C22	1.361(4)	.	.	no
C21	C26	1.365(4)	.	.	no
C22	C23	1.379(4)	.	.	no
C23	C24	1.385(4)	.	.	no
C24	C25	1.377(4)	.	.	no
C25	C26	1.381(4)	.	.	no
C6	H6'	0.980(9)	.	.	no
C6	H6	0.980(14)	.	.	no
C6	H6"	0.980(19)	.	.	no
C7	H7'	0.980(16)	.	.	no
C7	H7	0.980(11)	.	.	no
C7	H7"	0.980(10)	.	.	no
C8	H8'	0.981(8)	.	.	no
C8	H8"	0.980(10)	.	.	no
C8	H8	0.980(15)	.	.	no
C9	H9"	0.980(7)	.	.	no
C9	H9	0.979(16)	.	.	no
C9	H9'	0.981(16)	.	.	no
C10	H10"	0.980(10)	.	.	no
C10	H10	0.980(13)	.	.	no
C10	H10'	0.981(14)	.	.	no
C16	H16'	0.981(8)	.	.	no
C16	H16	0.980(14)	.	.	no
C16	H16"	0.980(15)	.	.	no
C17	H17'	0.980(19)	.	.	no
C17	H17	0.980(12)	.	.	no
C17	H17"	0.979(10)	.	.	no
C18	H18'	0.980(9)	.	.	no
C18	H18"	0.979(18)	.	.	no
C18	H18	0.98(2)	.	.	no
C19	H19'	0.982(19)	.	.	no
C19	H19"	0.98(2)	.	.	no
C19	H19	0.980(8)	.	.	no
C20	H20'	0.981(13)	.	.	no
C20	H20"	0.980(11)	.	.	no
C20	H20	0.980(7)	.	.	no
C22	H22	0.950(4)	.	.	no
C23	H23	0.950(4)	.	.	no
C24	H24	0.950(4)	.	.	no
C25	H25	0.949(4)	.	.	no
C26	H26	0.950(4)	.	.	no
C27	C32	1.401(3)	.	.	no
C27	C28	1.403(3)	.	.	no
C27	B	1.646(3)	.	.	yes
C28	C29	1.396(3)	.	.	no
C29	C30	1.385(4)	.	.	no
C30	C31	1.383(4)	.	.	no
C31	C32	1.389(3)	.	.	no
C33	C38	1.407(4)	.	.	no
C33	C34	1.397(3)	.	.	no
C33	B	1.640(3)	.	.	yes
C34	C35	1.396(4)	.	.	no
C35	C36	1.383(4)	.	.	no
C36	C37	1.392(4)	.	.	no
C37	C38	1.378(4)	.	.	no
C39	B	1.642(4)	.	.	yes
C39	C40	1.406(3)	.	.	no
C39	C44	1.397(3)	.	.	no
C40	C41	1.384(4)	.	.	no
C41	C42	1.387(4)	.	.	no
C42	C43	1.375(4)	.	.	no
C43	C44	1.392(4)	.	.	no
C45	C50	1.402(3)	.	.	no
C45	C46	1.406(4)	.	.	no
C45	B	1.639(3)	.	.	yes

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 C46     C47        1.383(4)                    .      .                 no
 C47     C48        1.384(4)                    .      .                 no
 C48     C49        1.377(4)                    .      .                 no
 C49     C50        1.393(4)                    .      .                 no
 C28     H28        0.950(3)                    .      .                 no
 C29     H29        0.950(4)                    .      .                 no
 C30     H30        0.950(4)                    .      .                 no
 C31     H31        0.950(4)                    .      .                 no
 C32     H32        0.950(3)                    .      .                 no
 C34     H34        0.950(4)                    .      .                 no
 C35     H35        0.950(4)                    .      .                 no
 C36     H36        0.950(4)                    .      .                 no
 C37     H37        0.950(4)                    .      .                 no
 C38     H38        0.950(4)                    .      .                 no
 C40     H40        0.950(4)                    .      .                 no
 C41     H41        0.951(4)                    .      .                 no
 C42     H42        0.950(4)                    .      .                 no
 C43     H43        0.950(4)                    .      .                 no
 C44     H44        0.950(4)                    .      .                 no
 C46     H46        0.950(4)                    .      .                 no
 C47     H47        0.950(4)                    .      .                 no
 C48     H48        0.950(4)                    .      .                 no
 C49     H49        0.950(4)                    .      .                 no
 C50     H50        0.950(4)                    .      .                 no
 C51     C56        1.374(5)                    .      .                 no
 C51     C52        1.368(4)                    .      .                 no
 C52     C53        1.381(4)                    .      .                 no
 C53     C54        1.378(4)                    .      .                 no
 C54     C55        1.373(4)                    .      .                 no
 C55     C56        1.383(4)                    .      .                 no
 C51     H51         0.95(5)                    .      .                 no
 C52     H52        0.949(4)                    .      .                 no
 C53     H53        0.950(4)                    .      .                 no
 C54     H54         0.95(5)                    .      .                 no
 C55     H55        0.950(4)                    .      .                 no
 C56     H56        0.950(4)                    .      .                 no

loop_
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_geom_angle_site_symmetry_3
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 F1      Ti1     C1        101.83(8)             .      .      .          yes
 F1      Ti1     C2        134.81(8)             .      .      .          yes
 F1      Ti1     C3        127.93(8)             .      .      .          yes
 F1      Ti1     C4         92.75(8)             .      .      .          yes
 F1      Ti1     C5         78.00(8)             .      .      .          yes
 F1      Ti1     C11       113.87(8)             .      .      .          yes
 F1      Ti1     C12       135.10(8)             .      .      .          yes
 F1      Ti1     C13       109.69(9)             .      .      .          yes
 F1      Ti1     C14        78.28(9)             .      .      .          yes
 F1      Ti1     C15        80.73(8)             .      .      .          yes
 C1      Ti1     C2         34.73(9)             .      .      .          yes
 C1      Ti1     C3         58.45(9)             .      .      .          yes
 C1      Ti1     C4        59.17(11)             .      .      .          yes
 C1      Ti1     C5        35.56(10)             .      .      .          yes
 C1      Ti1     C11       109.19(9)             .      .      .          yes
 C1      Ti1     C12       117.59(9)             .      .      .          yes
 C1      Ti1     C13      148.47(10)             .      .      .          yes
 C1      Ti1     C14      165.24(11)             .      .      .          yes
 C1      Ti1     C15       130.16(9)             .      .      .          yes
 C2      Ti1     C3         34.93(9)             .      .      .          yes
```

C2	Ti1	C4	58.45(9)	.	.	.	yes
C2	Ti1	C5	58.17(9)	.	.	.	yes
C2	Ti1	C11	97.64(9)	.	.	.	yes
C2	Ti1	C12	89.04(9)	.	.	.	yes
C2	Ti1	C13	114.32(9)	.	.	.	yes
C2	Ti1	C14	146.86(10)	.	.	.	yes
C2	Ti1	C15	131.73(9)	.	.	.	yes
C3	Ti1	C4	35.18(9)	.	.	.	yes
C3	Ti1	C5	58.45(10)	.	.	.	yes
C3	Ti1	C11	118.11(9)	.	.	.	yes
C3	Ti1	C12	92.47(9)	.	.	.	yes
C3	Ti1	C13	99.50(9)	.	.	.	yes
C3	Ti1	C14	132.91(11)	.	.	.	yes
C3	Ti1	C15	150.37(9)	.	.	.	yes
C4	Ti1	C5	35.48(13)	.	.	.	yes
C4	Ti1	C11	153.16(10)	.	.	.	yes
C4	Ti1	C12	124.89(10)	.	.	.	yes
C4	Ti1	C13	117.05(11)	.	.	.	yes
C4	Ti1	C14	135.52(12)	.	.	.	yes
C4	Ti1	C15	169.44(10)	.	.	.	yes
C5	Ti1	C11	143.85(11)	.	.	.	yes
C5	Ti1	C12	146.87(9)	.	.	.	yes
C5	Ti1	C13	152.51(11)	.	.	.	yes
C5	Ti1	C14	153.67(10)	.	.	.	yes
C5	Ti1	C15	147.96(11)	.	.	.	yes
C11	Ti1	C12	34.94(9)	.	.	.	yes
C11	Ti1	C13	58.65(9)	.	.	.	yes
C11	Ti1	C14	58.52(10)	.	.	.	yes
C11	Ti1	C15	35.12(9)	.	.	.	yes
C12	Ti1	C13	35.03(9)	.	.	.	yes
C12	Ti1	C14	58.07(10)	.	.	.	yes
C12	Ti1	C15	57.99(9)	.	.	.	yes
C13	Ti1	C14	35.13(11)	.	.	.	yes
C13	Ti1	C15	58.46(9)	.	.	.	yes
C14	Ti1	C15	35.09(11)	.	.	.	yes
Ti1	F1	C21	168.17(16)	.	.	.	yes
Ti1	C1	C2	74.48(15)	.	.	.	yes
Ti1	C1	C5	72.02(15)	.	.	.	yes
Ti1	C1	C6	123.6(2)	.	.	.	yes
C2	C1	C5	107.9(2)	.	.	.	no
C2	C1	C6	126.0(3)	.	.	.	no
C5	C1	C6	125.8(3)	.	.	.	no
Ti1	C2	C1	70.78(15)	.	.	.	yes
Ti1	C2	C3	71.93(14)	.	.	.	yes
Ti1	C2	C7	130.96(18)	.	.	.	yes
C1	C2	C3	108.2(2)	.	.	.	no
C1	C2	C7	125.0(3)	.	.	.	no
C3	C2	C7	126.0(2)	.	.	.	no
Ti1	C3	C2	73.14(15)	.	.	.	yes
Ti1	C3	C4	70.99(15)	.	.	.	yes
Ti1	C3	C8	128.45(18)	.	.	.	yes
C2	C3	C4	107.9(2)	.	.	.	no
C2	C3	C8	126.7(2)	.	.	.	no
C4	C3	C8	124.8(3)	.	.	.	no
Ti1	C4	C3	73.82(15)	.	.	.	yes
Ti1	C4	C5	72.25(16)	.	.	.	yes
Ti1	C4	C9	119.88(18)	.	.	.	yes
C3	C4	C5	107.7(3)	.	.	.	no
C3	C4	C9	125.1(3)	.	.	.	no
C5	C4	C9	127.2(3)	.	.	.	no
Ti1	C5	C1	72.42(15)	.	.	.	yes
Ti1	C5	C4	72.28(15)	.	.	.	yes
Ti1	C5	C10	125.57(18)	.	.	.	yes
C1	C5	C4	108.2(2)	.	.	.	no
C1	C5	C10	124.5(3)	.	.	.	no
C4	C5	C10	127.1(3)	.	.	.	no

Ti1	C11	C12	73.56(15)	.	.	.	yes
Ti1	C11	C15	72.57(15)	.	.	.	yes
Ti1	C11	C16	125.1(2)	.	.	.	yes
C12	C11	C15	107.8(2)	.	.	.	no
C12	C11	C16	127.1(3)	.	.	.	no
C15	C11	C16	124.7(3)	.	.	.	no
Ti1	C12	C11	71.50(15)	.	.	.	yes
Ti1	C12	C13	71.43(15)	.	.	.	yes
Ti1	C12	C17	132.8(2)	.	.	.	yes
C11	C12	C13	108.2(2)	.	.	.	no
C11	C12	C17	125.3(3)	.	.	.	no
C13	C12	C17	125.3(3)	.	.	.	no
Ti1	C13	C12	73.54(15)	.	.	.	yes
Ti1	C13	C14	72.65(16)	.	.	.	yes
Ti1	C13	C18	125.9(2)	.	.	.	yes
C12	C13	C14	107.8(2)	.	.	.	no
C12	C13	C18	125.7(3)	.	.	.	no
C14	C13	C18	126.0(3)	.	.	.	no
Ti1	C14	C13	72.23(15)	.	.	.	yes
Ti1	C14	C15	72.41(16)	.	.	.	yes
Ti1	C14	C19	123.5(2)	.	.	.	yes
C13	C14	C15	108.0(2)	.	.	.	no
C13	C14	C19	124.9(3)	.	.	.	no
C15	C14	C19	127.0(3)	.	.	.	no
Ti1	C15	C11	72.31(14)	.	.	.	yes
Ti1	C15	C14	72.51(15)	.	.	.	yes
Ti1	C15	C20	122.53(18)	.	.	.	yes
C11	C15	C14	108.2(2)	.	.	.	no
C11	C15	C20	125.2(3)	.	.	.	no
C14	C15	C20	126.5(3)	.	.	.	no
F1	C21	C22	117.1(2)	.	.	.	yes
F1	C21	C26	117.5(2)	.	.	.	yes
C22	C21	C26	125.4(2)	.	.	.	no
C21	C22	C23	116.9(2)	.	.	.	no
C22	C23	C24	119.9(2)	.	.	.	no
C23	C24	C25	120.8(2)	.	.	.	no
C24	C25	C26	120.1(2)	.	.	.	no
C21	C26	C25	116.8(2)	.	.	.	no
C1	C6	H6	109.4(6)	.	.	.	no
C1	C6	H6'	109.4(10)	.	.	.	no
C1	C6	H6"	109.4(7)	.	.	.	no
H6	C6	H6'	109.5(19)	.	.	.	no
H6	C6	H6"	109.5(16)	.	.	.	no
H6'	C6	H6"	109.5(19)	.	.	.	no
C2	C7	H7	109.5(5)	.	.	.	no
C2	C7	H7'	109.5(3)	.	.	.	no
C2	C7	H7"	109.4(4)	.	.	.	no
H7	C7	H7'	109.5(14)	.	.	.	no
H7	C7	H7"	109.5(16)	.	.	.	no
H7'	C7	H7"	109.5(15)	.	.	.	no
C3	C8	H8	109.5(5)	.	.	.	no
C3	C8	H8'	109.5(7)	.	.	.	no
C3	C8	H8"	109.5(5)	.	.	.	no
H8	C8	H8'	109.4(15)	.	.	.	no
H8	C8	H8"	109.5(12)	.	.	.	no
H8'	C8	H8"	109.4(13)	.	.	.	no
C4	C9	H9	109.5(10)	.	.	.	no
C4	C9	H9'	109.6(10)	.	.	.	no
C4	C9	H9"	109.5(5)	.	.	.	no
H9	C9	H9'	109.4(15)	.	.	.	no
H9	C9	H9"	109.5(15)	.	.	.	no
H9'	C9	H9"	109.4(15)	.	.	.	no
C5	C10	H10	109.4(7)	.	.	.	no
C5	C10	H10'	109.4(9)	.	.	.	no
C5	C10	H10"	109.5(8)	.	.	.	no
H10	C10	H10'	109.4(15)	.	.	.	no

H10	C10	H10"	109.5(17)	.	.	.	no
H10'	C10	H10"	109.5(13)	.	.	.	no
C11	C16	H16	109.4(9)	.	.	.	no
C11	C16	H16'	109.6(14)	.	.	.	no
C11	C16	H16"	109.4(9)	.	.	.	no
H16	C16	H16'	109.6(17)	.	.	.	no
H16	C16	H16"	109.5(15)	.	.	.	no
H16'	C16	H16"	109.3(19)	.	.	.	no
C12	C17	H17	109.5(5)	.	.	.	no
C12	C17	H17'	109.5(5)	.	.	.	no
C12	C17	H17"	109.5(7)	.	.	.	no
H17	C17	H17'	109.5(16)	.	.	.	no
H17	C17	H17"	109.5(17)	.	.	.	no
H17'	C17	H17"	109.5(17)	.	.	.	no
C13	C18	H18	109.5(6)	.	.	.	no
C13	C18	H18'	109.4(9)	.	.	.	no
C13	C18	H18"	109.6(7)	.	.	.	no
H18	C18	H18'	109.6(19)	.	.	.	no
H18	C18	H18"	109.5(18)	.	.	.	no
H18'	C18	H18"	109(2)	.	.	.	no
C14	C19	H19	109.5(6)	.	.	.	no
C14	C19	H19'	109.6(7)	.	.	.	no
C14	C19	H19"	109.5(8)	.	.	.	no
H19	C19	H19'	110(2)	.	.	.	no
H19	C19	H19"	109.6(16)	.	.	.	no
H19'	C19	H19"	109(2)	.	.	.	no
C15	C20	H20	109.5(9)	.	.	.	no
C15	C20	H20'	109.5(10)	.	.	.	no
C15	C20	H20"	109.5(10)	.	.	.	no
H20	C20	H20'	109.4(16)	.	.	.	no
H20	C20	H20"	109.5(19)	.	.	.	no
H20'	C20	H20"	109.4(13)	.	.	.	no
C21	C22	H22	121.5(3)	.	.	.	no
C23	C22	H22	121.6(3)	.	.	.	no
C22	C23	H23	120.1(3)	.	.	.	no
C24	C23	H23	120.0(3)	.	.	.	no
C23	C24	H24	119.7(3)	.	.	.	no
C25	C24	H24	119.5(3)	.	.	.	no
C24	C25	H25	120.0(3)	.	.	.	no
C26	C25	H25	119.9(3)	.	.	.	no
C21	C26	H26	121.6(3)	.	.	.	no
C25	C26	H26	121.6(3)	.	.	.	no
C28	C27	C32	115.5(2)	.	.	.	no
C28	C27	B	124.7(2)	.	.	.	yes
C32	C27	B	119.7(2)	.	.	.	yes
C27	C28	C29	122.4(2)	.	.	.	no
C28	C29	C30	120.0(2)	.	.	.	no
C29	C30	C31	119.2(2)	.	.	.	no
C30	C31	C32	120.1(2)	.	.	.	no
C27	C32	C31	122.8(2)	.	.	.	no
C34	C33	C38	114.6(2)	.	.	.	no
C34	C33	B	125.2(2)	.	.	.	yes
C38	C33	B	120.0(2)	.	.	.	yes
C33	C34	C35	123.0(2)	.	.	.	no
C34	C35	C36	120.3(2)	.	.	.	no
C35	C36	C37	118.5(2)	.	.	.	no
C36	C37	C38	120.2(2)	.	.	.	no
C33	C38	C37	123.5(2)	.	.	.	no
C40	C39	C44	114.7(2)	.	.	.	no
C40	C39	B	119.7(2)	.	.	.	yes
C44	C39	B	125.6(2)	.	.	.	yes
C39	C40	C41	123.1(2)	.	.	.	no
C40	C41	C42	119.9(2)	.	.	.	no
C41	C42	C43	119.0(2)	.	.	.	no
C42	C43	C44	120.3(2)	.	.	.	no
C39	C44	C43	122.9(2)	.	.	.	no

C46	C45	C50	115.0(2)	.	.	.	no
C46	C45	B	119.2(2)	.	.	.	yes
C50	C45	B	125.8(2)	.	.	.	yes
C45	C46	C47	122.9(2)	.	.	.	no
C46	C47	C48	120.3(3)	.	.	.	no
C47	C48	C49	118.8(3)	.	.	.	no
C48	C49	C50	120.5(3)	.	.	.	no
C45	C50	C49	122.4(2)	.	.	.	no
C29	C28	H28	118.8(3)	.	.	.	no
C27	C28	H28	118.8(3)	.	.	.	no
C28	C29	H29	120.0(3)	.	.	.	no
C30	C29	H29	120.0(3)	.	.	.	no
C31	C30	H30	120.4(3)	.	.	.	no
C29	C30	H30	120.4(3)	.	.	.	no
C30	C31	H31	120.0(3)	.	.	.	no
C32	C31	H31	120.0(3)	.	.	.	no
C27	C32	H32	118.6(3)	.	.	.	no
C31	C32	H32	118.6(3)	.	.	.	no
C35	C34	H34	118.5(3)	.	.	.	no
C33	C34	H34	118.5(3)	.	.	.	no
C34	C35	H35	119.8(3)	.	.	.	no
C36	C35	H35	119.9(3)	.	.	.	no
C35	C36	H36	120.8(3)	.	.	.	no
C37	C36	H36	120.7(3)	.	.	.	no
C38	C37	H37	119.9(3)	.	.	.	no
C36	C37	H37	119.9(3)	.	.	.	no
C33	C38	H38	118.2(3)	.	.	.	no
C37	C38	H38	118.3(3)	.	.	.	no
C39	C40	H40	118.4(3)	.	.	.	no
C41	C40	H40	118.4(3)	.	.	.	no
C42	C41	H41	120.1(3)	.	.	.	no
C40	C41	H41	120.0(3)	.	.	.	no
C41	C42	H42	120.5(3)	.	.	.	no
C43	C42	H42	120.6(3)	.	.	.	no
C44	C43	H43	119.9(3)	.	.	.	no
C42	C43	H43	119.9(3)	.	.	.	no
C39	C44	H44	118.5(3)	.	.	.	no
C43	C44	H44	118.6(3)	.	.	.	no
C45	C46	H46	118.6(3)	.	.	.	no
C47	C46	H46	118.5(3)	.	.	.	no
C48	C47	H47	119.8(3)	.	.	.	no
C46	C47	H47	119.9(3)	.	.	.	no
C47	C48	H48	120.6(4)	.	.	.	no
C49	C48	H48	120.6(3)	.	.	.	no
C48	C49	H49	119.7(3)	.	.	.	no
C50	C49	H49	119.7(4)	.	.	.	no
C49	C50	H50	118.8(3)	.	.	.	no
C45	C50	H50	118.8(3)	.	.	.	no
F2	C51	C56	117.5(3)	.	.	.	yes
C52	C51	C56	123.0(3)	.	.	.	no
F2	C51	C52	119.4(3)	.	.	.	yes
C51	C52	C53	118.5(3)	.	.	.	no
C52	C53	C54	119.0(3)	.	.	.	no
C53	C54	C55	121.9(3)	.	.	.	no
F21	C54	C55	119.1(4)	.	.	.	yes
F21	C54	C53	118.7(4)	.	.	.	yes
C54	C55	C56	119.2(3)	.	.	.	no
C51	C56	C55	118.2(3)	.	.	.	no
C56	C51	H51	116(7)	.	.	.	no
C52	C51	H51	113(7)	.	.	.	no
C51	C52	H52	120.7(3)	.	.	.	no
C53	C52	H52	120.7(3)	.	.	.	no
C52	C53	H53	120.5(3)	.	.	.	no
C54	C53	H53	120.5(3)	.	.	.	no
C55	C54	H54	120(4)	.	.	.	no
C53	C54	H54	116(4)	.	.	.	no

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 C56     C55     H55        120.5(3)              .       .       .          no
 C54     C55     H55        120.3(3)              .       .       .          no
 C55     C56     H56        120.9(4)              .       .       .          no
 C51     C56     H56        120.8(3)              .       .       .          no
 C39     B       C45      106.94(19)              .       .       .          yes
 C27     B       C33      103.56(18)              .       .       .          yes
 C27     B       C39      112.05(18)              .       .       .          yes
 C27     B       C45      109.82(18)              .       .       .          yes
 C33     B       C39      111.11(19)              .       .       .          yes
 C33     B       C45      113.47(19)              .       .       .          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
 F1      Ti1     C1      C2      -164.06(15)     .       .       .       .   no
 F1      Ti1     C1      C5       -48.83(18)     .       .       .       .   no
 F1      Ti1     C1      C6          72.7(3)     .       .       .       .   no
 C2      Ti1     C1      C5         115.2(2)     .       .       .       .   no
 C2      Ti1     C1      C6        -123.3(3)     .       .       .       .   no
 C3      Ti1     C1      C2       -36.59(15)     .       .       .       .   no
 C3      Ti1     C1      C5        78.64(18)     .       .       .       .   no
 C3      Ti1     C1      C6        -159.9(3)     .       .       .       .   no
 C4      Ti1     C1      C2       -77.96(17)     .       .       .       .   no
 C4      Ti1     C1      C5        37.26(17)     .       .       .       .   no
 C4      Ti1     C1      C6         158.8(3)     .       .       .       .   no
 C5      Ti1     C1      C2        -115.2(2)     .       .       .       .   no
 C5      Ti1     C1      C6         121.5(3)     .       .       .       .   no
 C11     Ti1     C1      C2        75.23(16)     .       .       .       .   no
 C11     Ti1     C1      C5      -169.54(17)     .       .       .       .   no
 C11     Ti1     C1      C6         -48.0(3)     .       .       .       .   no
 C12     Ti1     C1      C2        38.12(18)     .       .       .       .   no
 C12     Ti1     C1      C5       153.35(17)     .       .       .       .   no
 C12     Ti1     C1      C6         -85.2(3)     .       .       .       .   no
 C13     Ti1     C1      C2          14.3(3)     .       .       .       .   no
 C13     Ti1     C1      C5         129.6(2)     .       .       .       .   no
 C13     Ti1     C1      C6        -108.9(3)     .       .       .       .   no
 C15     Ti1     C1      C2       108.14(17)     .       .       .       .   no
 C15     Ti1     C1      C5      -136.63(18)     .       .       .       .   no
 C15     Ti1     C1      C6         -15.1(3)     .       .       .       .   no
 F1      Ti1     C2      C1          22.3(2)     .       .       .       .   no
 F1      Ti1     C2      C3       -95.22(17)     .       .       .       .   no
 F1      Ti1     C2      C7         142.4(2)     .       .       .       .   no
 C1      Ti1     C2      C3        -117.5(2)     .       .       .       .   no
 C1      Ti1     C2      C7         120.2(3)     .       .       .       .   no
 C3      Ti1     C2      C1         117.5(2)     .       .       .       .   no
 C3      Ti1     C2      C7        -122.4(3)     .       .       .       .   no
 C4      Ti1     C2      C1        80.21(18)     .       .       .       .   no
 C4      Ti1     C2      C3       -37.27(16)     .       .       .       .   no
 C4      Ti1     C2      C7        -159.6(3)     .       .       .       .   no
 C5      Ti1     C2      C1        38.25(17)     .       .       .       .   no
 C5      Ti1     C2      C3       -79.23(17)     .       .       .       .   no
 C5      Ti1     C2      C7         158.4(3)     .       .       .       .   no
 C11     Ti1     C2      C1      -112.86(16)     .       .       .       .   no
 C11     Ti1     C2      C3       129.66(15)     .       .       .       .   no
 C11     Ti1     C2      C7           7.3(3)     .       .       .       .   no
 C12     Ti1     C2      C1      -146.83(16)     .       .       .       .   no
 C12     Ti1     C2      C3        95.69(15)     .       .       .       .   no
 C12     Ti1     C2      C7         -26.7(3)     .       .       .       .   no
```

C13	Ti1	C2	C1	-171.84(15)	.	.	.	.	no
C13	Ti1	C2	C3	70.68(16)	.	.	.	.	no
C13	Ti1	C2	C7	-51.7(3)	.	.	.	.	no
C14	Ti1	C2	C1	-153.6(2)	.	.	.	.	no
C14	Ti1	C2	C3	89.0(2)	.	.	.	.	no
C14	Ti1	C2	C7	-33.4(4)	.	.	.	.	no
C15	Ti1	C2	C1	-103.31(17)	.	.	.	.	no
C15	Ti1	C2	C3	139.21(15)	.	.	.	.	no
C15	Ti1	C2	C7	16.8(3)	.	.	.	.	no
F1	Ti1	C3	C2	116.39(15)	.	.	.	.	no
F1	Ti1	C3	C4	0.0(2)	.	.	.	.	no
F1	Ti1	C3	C8	-119.8(2)	.	.	.	.	no
C1	Ti1	C3	C2	36.38(15)	.	.	.	.	no
C1	Ti1	C3	C4	-80.04(19)	.	.	.	.	no
C1	Ti1	C3	C8	160.2(3)	.	.	.	.	no
C2	Ti1	C3	C4	-116.4(2)	.	.	.	.	no
C2	Ti1	C3	C8	123.8(3)	.	.	.	.	no
C4	Ti1	C3	C2	116.4(2)	.	.	.	.	no
C4	Ti1	C3	C8	-119.8(3)	.	.	.	.	no
C5	Ti1	C3	C2	78.37(17)	.	.	.	.	no
C5	Ti1	C3	C4	-38.05(19)	.	.	.	.	no
C5	Ti1	C3	C8	-157.8(3)	.	.	.	.	no
C11	Ti1	C3	C2	-59.89(17)	.	.	.	.	no
C11	Ti1	C3	C4	-176.31(18)	.	.	.	.	no
C11	Ti1	C3	C8	63.9(3)	.	.	.	.	no
C12	Ti1	C3	C2	-84.78(15)	.	.	.	.	no
C12	Ti1	C3	C4	158.80(19)	.	.	.	.	no
C12	Ti1	C3	C8	39.0(2)	.	.	.	.	no
C13	Ti1	C3	C2	-119.32(15)	.	.	.	.	no
C13	Ti1	C3	C4	124.26(19)	.	.	.	.	no
C13	Ti1	C3	C8	4.5(2)	.	.	.	.	no
C14	Ti1	C3	C2	-131.73(16)	.	.	.	.	no
C14	Ti1	C3	C4	111.9(2)	.	.	.	.	no
C14	Ti1	C3	C8	-7.9(3)	.	.	.	.	no
C15	Ti1	C3	C2	-80.4(2)	.	.	.	.	no
C15	Ti1	C3	C4	163.1(2)	.	.	.	.	no
C15	Ti1	C3	C8	43.4(3)	.	.	.	.	no
F1	Ti1	C4	C3	179.98(17)	.	.	.	.	no
F1	Ti1	C4	C5	64.79(15)	.	.	.	.	no
F1	Ti1	C4	C9	-58.4(2)	.	.	.	.	no
C1	Ti1	C4	C3	77.83(17)	.	.	.	.	no
C1	Ti1	C4	C5	-37.35(15)	.	.	.	.	no
C1	Ti1	C4	C9	-160.6(3)	.	.	.	.	no
C2	Ti1	C4	C3	37.00(15)	.	.	.	.	no
C2	Ti1	C4	C5	-78.19(17)	.	.	.	.	no
C2	Ti1	C4	C9	158.6(3)	.	.	.	.	no
C3	Ti1	C4	C5	-115.2(2)	.	.	.	.	no
C3	Ti1	C4	C9	121.6(3)	.	.	.	.	no
C5	Ti1	C4	C3	115.2(2)	.	.	.	.	no
C5	Ti1	C4	C9	-123.2(3)	.	.	.	.	no
C11	Ti1	C4	C3	7.2(3)	.	.	.	.	no
C11	Ti1	C4	C5	-108.0(2)	.	.	.	.	no
C11	Ti1	C4	C9	128.8(2)	.	.	.	.	no
C12	Ti1	C4	C3	-26.1(2)	.	.	.	.	no
C12	Ti1	C4	C5	-141.32(15)	.	.	.	.	no
C12	Ti1	C4	C9	95.5(2)	.	.	.	.	no
C13	Ti1	C4	C3	-66.24(19)	.	.	.	.	no
C13	Ti1	C4	C5	178.57(15)	.	.	.	.	no
C13	Ti1	C4	C9	55.3(3)	.	.	.	.	no
C14	Ti1	C4	C3	-104.00(19)	.	.	.	.	no
C14	Ti1	C4	C5	140.82(17)	.	.	.	.	no
C14	Ti1	C4	C9	17.6(3)	.	.	.	.	no
F1	Ti1	C5	C1	131.13(18)	.	.	.	.	no
F1	Ti1	C5	C4	-112.49(16)	.	.	.	.	no
F1	Ti1	C5	C10	10.9(3)	.	.	.	.	no
C1	Ti1	C5	C4	116.4(2)	.	.	.	.	no

C1	Ti1	C5	C10	-120.2(4)	.	.	.	.	no
C2	Ti1	C5	C1	-37.35(15)	.	.	.	.	no
C2	Ti1	C5	C4	79.04(16)	.	.	.	.	no
C2	Ti1	C5	C10	-157.6(3)	.	.	.	.	no
C3	Ti1	C5	C1	-78.66(17)	.	.	.	.	no
C3	Ti1	C5	C4	37.73(15)	.	.	.	.	no
C3	Ti1	C5	C10	161.1(3)	.	.	.	.	no
C4	Ti1	C5	C1	-116.4(2)	.	.	.	.	no
C4	Ti1	C5	C10	123.4(3)	.	.	.	.	no
C11	Ti1	C5	C1	16.9(3)	.	.	.	.	no
C11	Ti1	C5	C4	133.28(19)	.	.	.	.	no
C11	Ti1	C5	C10	-103.3(3)	.	.	.	.	no
C12	Ti1	C5	C1	-46.7(3)	.	.	.	.	no
C12	Ti1	C5	C4	69.7(3)	.	.	.	.	no
C12	Ti1	C5	C10	-166.9(2)	.	.	.	.	no
C13	Ti1	C5	C1	-119.1(2)	.	.	.	.	no
C13	Ti1	C5	C4	-2.8(3)	.	.	.	.	no
C13	Ti1	C5	C10	120.6(3)	.	.	.	.	no
C14	Ti1	C5	C1	157.3(2)	.	.	.	.	no
C14	Ti1	C5	C4	-86.4(3)	.	.	.	.	no
C14	Ti1	C5	C10	37.0(5)	.	.	.	.	no
C15	Ti1	C5	C1	81.7(2)	.	.	.	.	no
C15	Ti1	C5	C4	-161.96(18)	.	.	.	.	no
C15	Ti1	C5	C10	-38.6(4)	.	.	.	.	no
F1	Ti1	C11	C12	135.98(15)	.	.	.	.	no
F1	Ti1	C11	C15	20.76(17)	.	.	.	.	no
F1	Ti1	C11	C16	-99.9(3)	.	.	.	.	no
C1	Ti1	C11	C12	-110.98(16)	.	.	.	.	no
C1	Ti1	C11	C15	133.79(15)	.	.	.	.	no
C1	Ti1	C11	C16	13.2(3)	.	.	.	.	no
C2	Ti1	C11	C12	-77.21(16)	.	.	.	.	no
C2	Ti1	C11	C15	167.57(15)	.	.	.	.	no
C2	Ti1	C11	C16	46.9(3)	.	.	.	.	no
C3	Ti1	C11	C12	-47.22(18)	.	.	.	.	no
C3	Ti1	C11	C15	-162.45(14)	.	.	.	.	no
C3	Ti1	C11	C16	76.9(3)	.	.	.	.	no
C4	Ti1	C11	C12	-51.9(3)	.	.	.	.	no
C4	Ti1	C11	C15	-167.2(2)	.	.	.	.	no
C4	Ti1	C11	C16	72.2(4)	.	.	.	.	no
C5	Ti1	C11	C12	-121.29(19)	.	.	.	.	no
C5	Ti1	C11	C15	123.49(19)	.	.	.	.	no
C5	Ti1	C11	C16	2.9(3)	.	.	.	.	no
C12	Ti1	C11	C15	-115.2(2)	.	.	.	.	no
C12	Ti1	C11	C16	124.2(3)	.	.	.	.	no
C13	Ti1	C11	C12	36.67(15)	.	.	.	.	no
C13	Ti1	C11	C15	-78.55(16)	.	.	.	.	no
C13	Ti1	C11	C16	160.8(3)	.	.	.	.	no
C14	Ti1	C11	C12	78.08(17)	.	.	.	.	no
C14	Ti1	C11	C15	-37.14(16)	.	.	.	.	no
C14	Ti1	C11	C16	-157.8(3)	.	.	.	.	no
C15	Ti1	C11	C12	115.2(2)	.	.	.	.	no
C15	Ti1	C11	C16	-120.6(3)	.	.	.	.	no
F1	Ti1	C12	C11	-64.19(19)	.	.	.	.	no
F1	Ti1	C12	C13	53.1(2)	.	.	.	.	no
F1	Ti1	C12	C17	174.5(2)	.	.	.	.	no
C1	Ti1	C12	C11	84.24(17)	.	.	.	.	no
C1	Ti1	C12	C13	-158.44(15)	.	.	.	.	no
C1	Ti1	C12	C17	-37.1(3)	.	.	.	.	no
C2	Ti1	C12	C11	104.83(16)	.	.	.	.	no
C2	Ti1	C12	C13	-137.84(16)	.	.	.	.	no
C2	Ti1	C12	C17	-16.5(3)	.	.	.	.	no
C3	Ti1	C12	C11	139.61(16)	.	.	.	.	no
C3	Ti1	C12	C13	-103.07(16)	.	.	.	.	no
C3	Ti1	C12	C17	18.3(3)	.	.	.	.	no
C4	Ti1	C12	C11	154.32(16)	.	.	.	.	no
C4	Ti1	C12	C13	-88.35(18)	.	.	.	.	no

C4	Ti1	C12	C17	33.0(3)	.	.	.	no
C5	Ti1	C12	C11	112.7(2)	.	.	.	no
C5	Ti1	C12	C13	-129.9(2)	.	.	.	no
C5	Ti1	C12	C17	-8.6(4)	.	.	.	no
C11	Ti1	C12	C13	117.3(2)	.	.	.	no
C11	Ti1	C12	C17	-121.3(3)	.	.	.	no
C13	Ti1	C12	C11	-117.3(2)	.	.	.	no
C13	Ti1	C12	C17	121.3(3)	.	.	.	no
C14	Ti1	C12	C11	-79.49(18)	.	.	.	no
C14	Ti1	C12	C13	37.83(17)	.	.	.	no
C14	Ti1	C12	C17	159.2(3)	.	.	.	no
C15	Ti1	C12	C11	-37.86(15)	.	.	.	no
C15	Ti1	C12	C13	79.46(17)	.	.	.	no
C15	Ti1	C12	C17	-159.2(3)	.	.	.	no
F1	Ti1	C13	C12	-143.15(15)	.	.	.	no
F1	Ti1	C13	C14	-27.92(19)	.	.	.	no
F1	Ti1	C13	C18	94.4(3)	.	.	.	no
C1	Ti1	C13	C12	38.5(3)	.	.	.	no
C1	Ti1	C13	C14	153.8(2)	.	.	.	no
C1	Ti1	C13	C18	-84.0(3)	.	.	.	no
C2	Ti1	C13	C12	47.43(17)	.	.	.	no
C2	Ti1	C13	C14	162.66(17)	.	.	.	no
C2	Ti1	C13	C18	-75.1(3)	.	.	.	no
C3	Ti1	C13	C12	80.65(16)	.	.	.	no
C3	Ti1	C13	C14	-164.12(17)	.	.	.	no
C3	Ti1	C13	C18	-41.8(3)	.	.	.	no
C4	Ti1	C13	C12	112.97(16)	.	.	.	no
C4	Ti1	C13	C14	-131.80(17)	.	.	.	no
C4	Ti1	C13	C18	-9.5(3)	.	.	.	no
C5	Ti1	C13	C12	114.8(2)	.	.	.	no
C5	Ti1	C13	C14	-130.0(2)	.	.	.	no
C5	Ti1	C13	C18	-7.7(4)	.	.	.	no
C11	Ti1	C13	C12	-36.57(15)	.	.	.	no
C11	Ti1	C13	C14	78.66(18)	.	.	.	no
C11	Ti1	C13	C18	-159.1(3)	.	.	.	no
C12	Ti1	C13	C14	115.2(2)	.	.	.	no
C12	Ti1	C13	C18	-122.5(3)	.	.	.	no
C14	Ti1	C13	C12	-115.2(2)	.	.	.	no
C14	Ti1	C13	C18	122.3(3)	.	.	.	no
C15	Ti1	C13	C12	-78.00(16)	.	.	.	no
C15	Ti1	C13	C14	37.23(17)	.	.	.	no
C15	Ti1	C13	C18	159.5(3)	.	.	.	no
F1	Ti1	C14	C13	153.24(18)	.	.	.	no
F1	Ti1	C14	C15	-90.53(16)	.	.	.	no
F1	Ti1	C14	C19	32.7(3)	.	.	.	no
C2	Ti1	C14	C13	-29.8(3)	.	.	.	no
C2	Ti1	C14	C15	86.4(2)	.	.	.	no
C2	Ti1	C14	C19	-150.3(3)	.	.	.	no
C3	Ti1	C14	C13	21.6(2)	.	.	.	no
C3	Ti1	C14	C15	137.84(16)	.	.	.	no
C3	Ti1	C14	C19	-98.9(3)	.	.	.	no
C4	Ti1	C14	C13	71.4(2)	.	.	.	no
C4	Ti1	C14	C15	-172.40(16)	.	.	.	no
C4	Ti1	C14	C19	-49.2(4)	.	.	.	no
C5	Ti1	C14	C13	127.1(3)	.	.	.	no
C5	Ti1	C14	C15	-116.6(3)	.	.	.	no
C5	Ti1	C14	C19	6.6(5)	.	.	.	no
C11	Ti1	C14	C13	-79.05(17)	.	.	.	no
C11	Ti1	C14	C15	37.17(15)	.	.	.	no
C11	Ti1	C14	C19	160.4(4)	.	.	.	no
C12	Ti1	C14	C13	-37.72(15)	.	.	.	no
C12	Ti1	C14	C15	78.50(17)	.	.	.	no
C12	Ti1	C14	C19	-158.3(4)	.	.	.	no
C13	Ti1	C14	C15	116.2(2)	.	.	.	no
C13	Ti1	C14	C19	-120.5(4)	.	.	.	no
C15	Ti1	C14	C13	-116.2(2)	.	.	.	no

C15	Ti1	C14	C19	123.2(4)	.	.	.	no
F1	Ti1	C15	C11	-160.83(16)	.	.	.	no
F1	Ti1	C15	C14	82.77(16)	.	.	.	no
F1	Ti1	C15	C20	-39.9(2)	.	.	.	no
C1	Ti1	C15	C11	-63.12(19)	.	.	.	no
C1	Ti1	C15	C14	-179.53(16)	.	.	.	no
C1	Ti1	C15	C20	57.8(3)	.	.	.	no
C2	Ti1	C15	C11	-16.6(2)	.	.	.	no
C2	Ti1	C15	C14	-133.02(17)	.	.	.	no
C2	Ti1	C15	C20	104.4(3)	.	.	.	no
C3	Ti1	C15	C11	32.6(3)	.	.	.	no
C3	Ti1	C15	C14	-83.9(2)	.	.	.	no
C3	Ti1	C15	C20	153.5(2)	.	.	.	no
C5	Ti1	C15	C11	-112.0(2)	.	.	.	no
C5	Ti1	C15	C14	131.6(2)	.	.	.	no
C5	Ti1	C15	C20	9.0(3)	.	.	.	no
C11	Ti1	C15	C14	-116.4(2)	.	.	.	no
C11	Ti1	C15	C20	121.0(3)	.	.	.	no
C12	Ti1	C15	C11	37.66(15)	.	.	.	no
C12	Ti1	C15	C14	-78.74(17)	.	.	.	no
C12	Ti1	C15	C20	158.6(3)	.	.	.	no
C13	Ti1	C15	C11	79.13(16)	.	.	.	no
C13	Ti1	C15	C14	-37.27(16)	.	.	.	no
C13	Ti1	C15	C20	-159.9(3)	.	.	.	no
C14	Ti1	C15	C11	116.4(2)	.	.	.	no
C14	Ti1	C15	C20	-122.6(3)	.	.	.	no
Ti1	C1	C2	C3	62.59(18)	.	.	.	no
Ti1	C1	C2	C7	-127.1(3)	.	.	.	no
C5	C1	C2	Ti1	-64.75(18)	.	.	.	no
C5	C1	C2	C3	-2.2(3)	.	.	.	no
C5	C1	C2	C7	168.1(2)	.	.	.	no
C6	C1	C2	Ti1	120.5(3)	.	.	.	no
C6	C1	C2	C3	-176.9(3)	.	.	.	no
C6	C1	C2	C7	-6.6(5)	.	.	.	no
Ti1	C1	C5	C4	-63.90(18)	.	.	.	no
Ti1	C1	C5	C10	121.5(2)	.	.	.	no
C2	C1	C5	Ti1	66.38(19)	.	.	.	no
C2	C1	C5	C4	2.5(3)	.	.	.	no
C2	C1	C5	C10	-172.1(2)	.	.	.	no
C6	C1	C5	Ti1	-118.8(3)	.	.	.	no
C6	C1	C5	C4	177.3(3)	.	.	.	no
C6	C1	C5	C10	2.7(4)	.	.	.	no
Ti1	C2	C3	C4	62.88(17)	.	.	.	no
Ti1	C2	C3	C8	-125.8(3)	.	.	.	no
C1	C2	C3	Ti1	-61.86(19)	.	.	.	no
C1	C2	C3	C4	1.0(3)	.	.	.	no
C1	C2	C3	C8	172.4(2)	.	.	.	no
C7	C2	C3	Ti1	128.0(3)	.	.	.	no
C7	C2	C3	C4	-169.1(2)	.	.	.	no
C7	C2	C3	C8	2.2(4)	.	.	.	no
Ti1	C3	C4	C5	64.79(18)	.	.	.	no
Ti1	C3	C4	C9	-115.5(3)	.	.	.	no
C2	C3	C4	Ti1	-64.27(18)	.	.	.	no
C2	C3	C4	C5	0.5(3)	.	.	.	no
C2	C3	C4	C9	-179.8(2)	.	.	.	no
C8	C3	C4	Ti1	124.2(2)	.	.	.	no
C8	C3	C4	C5	-171.0(2)	.	.	.	no
C8	C3	C4	C9	8.7(4)	.	.	.	no
Ti1	C4	C5	C1	63.99(18)	.	.	.	no
Ti1	C4	C5	C10	-121.6(3)	.	.	.	no
C3	C4	C5	Ti1	-65.83(17)	.	.	.	no
C3	C4	C5	C1	-1.8(3)	.	.	.	no
C3	C4	C5	C10	172.6(2)	.	.	.	no
C9	C4	C5	Ti1	114.4(3)	.	.	.	no
C9	C4	C5	C1	178.4(2)	.	.	.	no
C9	C4	C5	C10	-7.2(4)	.	.	.	no

Ti1	C11	C12	C13	-62.41(19)	.	.	.	.	no
Ti1	C11	C12	C17	129.8(3)	.	.	.	.	no
C15	C11	C12	Ti1	65.00(18)	.	.	.	.	no
C15	C11	C12	C13	2.6(3)	.	.	.	.	no
C15	C11	C12	C17	-165.2(3)	.	.	.	.	no
C16	C11	C12	Ti1	-122.0(3)	.	.	.	.	no
C16	C11	C12	C13	175.6(3)	.	.	.	.	no
C16	C11	C12	C17	7.9(5)	.	.	.	.	no
Ti1	C11	C15	C14	64.07(18)	.	.	.	.	no
Ti1	C11	C15	C20	-117.8(3)	.	.	.	.	no
C12	C11	C15	Ti1	-65.66(18)	.	.	.	.	no
C12	C11	C15	C14	-1.6(3)	.	.	.	.	no
C12	C11	C15	C20	176.6(2)	.	.	.	.	no
C16	C11	C15	Ti1	121.1(3)	.	.	.	.	no
C16	C11	C15	C14	-174.8(3)	.	.	.	.	no
C16	C11	C15	C20	3.3(4)	.	.	.	.	no
Ti1	C12	C13	C14	-65.07(19)	.	.	.	.	no
Ti1	C12	C13	C18	122.8(3)	.	.	.	.	no
C11	C12	C13	Ti1	62.46(18)	.	.	.	.	no
C11	C12	C13	C14	-2.6(3)	.	.	.	.	no
C11	C12	C13	C18	-174.8(3)	.	.	.	.	no
C17	C12	C13	Ti1	-129.8(3)	.	.	.	.	no
C17	C12	C13	C14	165.1(3)	.	.	.	.	no
C17	C12	C13	C18	-7.1(5)	.	.	.	.	no
Ti1	C13	C14	C15	-64.03(19)	.	.	.	.	no
Ti1	C13	C14	C19	118.8(3)	.	.	.	.	no
C12	C13	C14	Ti1	65.67(19)	.	.	.	.	no
C12	C13	C14	C15	1.6(3)	.	.	.	.	no
C12	C13	C14	C19	-175.5(3)	.	.	.	.	no
C18	C13	C14	Ti1	-122.2(3)	.	.	.	.	no
C18	C13	C14	C15	173.8(3)	.	.	.	.	no
C18	C13	C14	C19	-3.4(5)	.	.	.	.	no
Ti1	C14	C15	C11	-63.95(18)	.	.	.	.	no
Ti1	C14	C15	C20	117.9(3)	.	.	.	.	no
C13	C14	C15	Ti1	63.92(19)	.	.	.	.	no
C13	C14	C15	C11	0.0(3)	.	.	.	.	no
C13	C14	C15	C20	-178.2(2)	.	.	.	.	no
C19	C14	C15	Ti1	-119.0(3)	.	.	.	.	no
C19	C14	C15	C11	177.0(3)	.	.	.	.	no
C19	C14	C15	C20	-1.1(5)	.	.	.	.	no
F1	C21	C22	C23	178.7(2)	.	.	.	.	no
C26	C21	C22	C23	-0.2(4)	.	.	.	.	no
F1	C21	C26	C25	-179.6(2)	.	.	.	.	no
C22	C21	C26	C25	-0.6(4)	.	.	.	.	no
C21	C22	C23	C24	0.7(4)	.	.	.	.	no
C22	C23	C24	C25	-0.4(4)	.	.	.	.	no
C23	C24	C25	C26	-0.4(4)	.	.	.	.	no
C24	C25	C26	C21	0.9(4)	.	.	.	.	no
C32	C27	C28	C29	1.6(4)	.	.	.	.	no
B	C27	C28	C29	178.9(2)	.	.	.	.	no
C28	C27	C32	C31	-2.2(4)	.	.	.	.	no
B	C27	C32	C31	-179.6(2)	.	.	.	.	no
C32	C27	B	C39	-53.7(3)	.	.	.	.	no
C28	C27	B	C45	10.5(3)	.	.	.	.	no
C32	C27	B	C45	-172.4(2)	.	.	.	.	no
C28	C27	B	C33	-111.0(3)	.	.	.	.	no
C32	C27	B	C33	66.1(3)	.	.	.	.	no
C28	C27	B	C39	129.1(2)	.	.	.	.	no
C27	C28	C29	C30	-0.1(4)	.	.	.	.	no
C28	C29	C30	C31	-1.0(4)	.	.	.	.	no
C29	C30	C31	C32	0.4(4)	.	.	.	.	no
C30	C31	C32	C27	1.2(4)	.	.	.	.	no
B	C33	C34	C35	174.2(2)	.	.	.	.	no
C38	C33	C34	C35	0.4(4)	.	.	.	.	no
C34	C33	B	C27	-110.6(2)	.	.	.	.	no
C34	C33	C38	C37	-0.8(4)	.	.	.	.	no

```
 B       C33     C38     C37       -174.9(2)     .       .       .       .   no
 C38     C33     B       C45        -56.2(3)     .       .       .       .   no
 C34     C33     B       C45        130.4(2)     .       .       .       .   no
 C38     C33     B       C27         62.8(3)     .       .       .       .   no
 C34     C33     B       C39          9.8(3)     .       .       .       .   no
 C38     C33     B       C39       -176.7(2)     .       .       .       .   no
 C33     C34     C35     C36          0.3(4)     .       .       .       .   no
 C34     C35     C36     C37         -0.8(4)     .       .       .       .   no
 C35     C36     C37     C38          0.5(4)     .       .       .       .   no
 C36     C37     C38     C33          0.3(4)     .       .       .       .   no
 C44     C39     C40     C41          1.9(4)     .       .       .       .   no
 C40     C39     B       C27        170.2(2)     .       .       .       .   no
 C44     C39     B       C27        -12.2(3)     .       .       .       .   no
 C40     C39     B       C33         54.9(3)     .       .       .       .   no
 B       C39     C40     C41        179.8(2)     .       .       .       .   no
 C40     C39     C44     C43         -0.7(4)     .       .       .       .   no
 B       C39     C44     C43       -178.4(2)     .       .       .       .   no
 C44     C39     B       C45        108.2(3)     .       .       .       .   no
 C44     C39     B       C33       -127.5(2)     .       .       .       .   no
 C40     C39     B       C45        -69.4(3)     .       .       .       .   no
 C39     C40     C41     C42         -0.9(4)     .       .       .       .   no
 C40     C41     C42     C43         -1.4(4)     .       .       .       .   no
 C41     C42     C43     C44          2.6(4)     .       .       .       .   no
 C42     C43     C44     C39         -1.5(4)     .       .       .       .   no
 C50     C45     C46     C47          2.2(4)     .       .       .       .   no
 C46     C45     B       C27         61.9(3)     .       .       .       .   no
 C50     C45     B       C27       -118.2(3)     .       .       .       .   no
 C46     C45     B       C33        177.2(2)     .       .       .       .   no
 C50     C45     B       C33         -2.9(3)     .       .       .       .   no
 B       C45     C46     C47       -177.9(2)     .       .       .       .   no
 C46     C45     C50     C49         -1.2(4)     .       .       .       .   no
 B       C45     C50     C49        178.9(3)     .       .       .       .   no
 C46     C45     B       C39        -59.9(3)     .       .       .       .   no
 C50     C45     B       C39        120.0(3)     .       .       .       .   no
 C45     C46     C47     C48         -1.9(4)     .       .       .       .   no
 C46     C47     C48     C49          0.5(5)     .       .       .       .   no
 C47     C48     C49     C50          0.5(5)     .       .       .       .   no
 C48     C49     C50     C45         -0.1(5)     .       .       .       .   no
 F2      C51     C52     C53       -174.8(3)     .       .       .       .   no
 C56     C51     C52     C53          1.7(5)     .       .       .       .   no
 F2      C51     C56     C55        174.6(3)     .       .       .       .   no
 C52     C51     C56     C55         -2.0(5)     .       .       .       .   no
 C51     C52     C53     C54         -0.4(4)     .       .       .       .   no
 C52     C53     C54     C55         -0.6(5)     .       .       .       .   no
 C53     C54     C55     C56          0.3(5)     .       .       .       .   no
 C54     C55     C56     C51          1.0(5)     .       .       .       .   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     H19       3.605(18)                     .       .                 no
 Ti1     H19"      3.487(18)                     .       .                 no
 Ti1     H20         3.66(2)                     .       .                 no
 Ti1     H20'      3.431(14)                     .       .                 no
 F2      C6         3.334(5)                     .     2_666               no
 F21     C16        3.267(8)                     .     1_655               no
 F21     C35        3.288(7)                     .     1_545               no
 F21     F21        2.424(6)                     .     2_756               no
 F21     C36        3.317(6)                     .     2_766               no
 F21     C35        3.301(7)                     .     2_766               no
 F21     C36        3.350(6)                     .     1_545               no
 F1      H10"        2.79(2)                     .       .                 no
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F1	H19	2.63(2)	.	.	no
F1	H20	2.82(2)	.	.	no
F1	H10'	2.668(14)	.	.	no
F2	H7"	2.584(19)	.	2_666	no
F2	H31	2.474(4)	.	.	no
F2	H6'	2.74(2)	.	2_666	no
F21	H36	2.776(6)	.	1_545	no
F21	H35	2.633(7)	.	1_545	no
C6	F2	3.334(5)	.	2_666	no
C7	C17	3.356(5)	.	.	no
C9	C28	3.573(4)	.	.	no
C10	C21	3.239(4)	.	.	no
C16	F21	3.267(8)	.	1_455	no
C16	C54	3.553(5)	.	1_455	no
C17	C41	3.598(4)	.	2_666	no
C17	C42	3.581(4)	.	2_666	no
C17	C7	3.356(5)	.	.	no
C19	F1	3.003(5)	.	.	no
C19	C21	3.539(5)	.	.	no
C20	F1	3.139(4)	.	.	no
C21	C19	3.539(5)	.	.	no
C21	C10	3.239(4)	.	.	no
C22	C47	3.509(4)	.	2_565	no
C23	C42	3.512(4)	.	2_565	no
C23	C41	3.522(4)	.	2_565	no
C24	C42	3.524(4)	.	2_565	no
C25	C38	3.471(4)	.	2_665	no
C25	C37	3.589(4)	.	2_665	no
C26	C38	3.553(4)	.	2_665	no
C28	C46	3.234(4)	.	.	no
C28	C9	3.573(4)	.	.	no
C32	C44	3.219(4)	.	.	no
C34	C40	3.172(4)	.	.	no
C35	F21	3.301(7)	.	2_766	no
C35	F21	3.288(7)	.	1_565	no
C36	F21	3.317(6)	.	2_766	no
C36	F21	3.350(6)	.	1_565	no
C37	C49	3.597(4)	.	2_675	no
C37	C25	3.589(4)	.	2_665	no
C38	C26	3.553(4)	.	2_665	no
C38	C50	3.235(4)	.	.	no
C38	C25	3.471(4)	.	2_665	no
C40	C34	3.172(4)	.	.	no
C41	C17	3.598(4)	.	2_666	no
C41	C23	3.522(4)	.	2_565	no
C42	C17	3.581(4)	.	2_666	no
C42	C24	3.524(4)	.	2_565	no
C42	C23	3.512(4)	.	2_565	no
C44	C32	3.219(4)	.	.	no
C46	C28	3.234(4)	.	.	no
C47	C22	3.509(4)	.	2_565	no
C49	C37	3.597(4)	.	2_675	no
C50	C38	3.235(4)	.	.	no
C54	C16	3.553(5)	.	1_655	no
C6	H7'	2.972(11)	.	.	no
C6	H10'	2.939(16)	.	.	no
C7	H32	2.876(4)	.	2_666	no
C7	H6"	2.805(13)	.	.	no
C7	H17	2.73(2)	.	.	no
C7	H8	2.869(7)	.	.	no
C8	H18"	3.09(2)	.	.	no
C8	H7	2.823(10)	.	.	no
C8	H17'	2.92(2)	.	.	no
C8	H9	3.065(18)	.	.	no
C9	H10"	2.862(11)	.	.	no
C9	H8"	2.885(11)	.	.	no

C9	H44	3.055(4)	.	.	no
C10	H9"	2.836(6)	.	.	no
C10	H6	2.965(15)	.	.	no
C11	H41	2.823(4)	.	1_545	no
C13	H40	3.080(4)	.	1_545	no
C14	H40	3.011(4)	.	1_545	no
C16	H20'	2.96(2)	.	.	no
C16	H7'	3.060(15)	.	.	no
C16	H54	3.01(7)	.	1_455	no
C16	H17	2.867(12)	.	.	no
C17	H18"	2.805(13)	.	.	no
C17	H7	2.79(2)	.	.	no
C17	H8	2.943(17)	.	.	no
C17	H16	2.834(14)	.	.	no
C18	H17'	2.900(10)	.	.	no
C18	H8"	3.09(2)	.	.	no
C18	H19"	2.904(14)	.	.	no
C19	H18	2.978(17)	.	.	no
C19	H20	2.830(12)	.	.	no
C20	H16"	2.968(15)	.	.	no
C20	H19	2.860(8)	.	.	no
C21	H10"	2.82(2)	.	.	no
C21	H19	2.90(2)	.	.	no
C21	H10'	2.923(15)	.	.	no
C23	H10	3.053(11)	.	2_565	no
C24	H10	2.900(13)	.	2_565	no
C26	H38	2.937(4)	.	2_665	no
C26	H10"	2.953(19)	.	.	no
C27	H44	2.721(4)	.	.	no
C27	H46	3.048(4)	.	.	no
C27	H9'	2.857(17)	.	.	no
C27	H38	2.983(3)	.	.	no
C28	H9'	2.823(19)	.	.	no
C28	H26	2.989(4)	.	2_665	no
C29	H9'	3.09(2)	.	.	no
C30	H25	3.037(4)	.	2_665	no
C31	H52	3.093(4)	.	.	no
C31	H25	3.007(4)	.	2_665	no
C31	H56	2.857(4)	.	2_766	no
C32	H44	2.684(4)	.	.	no
C32	H25	3.090(4)	.	2_665	no
C33	H50	2.751(3)	.	.	no
C33	H32	3.001(3)	.	.	no
C33	H40	2.961(4)	.	.	no
C34	H18'	2.902(11)	.	1_565	no
C34	H40	2.917(4)	.	.	no
C35	H53	2.932(4)	.	1_565	no
C35	H55	2.869(4)	.	2_766	no
C35	H18'	3.016(16)	.	1_565	no
C36	H55	2.924(4)	.	2_766	no
C36	H53	3.001(4)	.	1_565	no
C37	H49	2.874(4)	.	2_675	no
C38	H49	3.055(4)	.	2_675	no
C38	H50	2.653(4)	.	.	no
C39	H23	3.026(4)	.	2_565	no
C39	H46	2.929(3)	.	.	no
C39	H32	2.967(4)	.	.	no
C39	H34	2.667(3)	.	.	no
C40	H34	2.585(4)	.	.	no
C40	H23	2.801(4)	.	2_565	no
C41	H23	2.747(4)	.	2_565	no
C42	H17'	2.946(11)	.	2_666	no
C42	H23	2.872(4)	.	2_565	no
C42	H24	2.889(4)	.	2_565	no
C43	H23	3.003(4)	.	2_565	no
C44	H9'	3.095(15)	.	.	no

C44	H32	2.952(4)	.	.	no
C44	H23	3.074(4)	.	2_565	no
C45	H38	3.006(4)	.	.	no
C45	H28	2.637(3)	.	.	no
C46	H28	2.712(4)	.	.	no
C47	H30	3.038(4)	.	2_665	no
C47	H22	2.738(4)	.	2_565	no
C49	H19'	3.012(17)	.	1_565	no
C49	H18	3.094(14)	.	2_665	no
C50	H19'	2.73(2)	.	1_565	no
C50	H38	2.894(4)	.	.	no
C52	H42	2.972(4)	.	2_666	no
C52	H31	3.067(4)	.	.	no
C53	H42	2.971(4)	.	2_666	no
C54	H16"	3.089(13)	.	1_655	no
C55	H24	3.099(4)	.	1_656	no
C56	H24	2.840(4)	.	1_656	no
H6	C10	2.965(15)	.	.	no
H6	H10'	2.46(2)	.	.	no
H6'	F2	2.74(2)	.	2_666	no
H6"	H7'	2.355(19)	.	.	no
H6"	C7	2.805(13)	.	.	no
H7	C8	2.823(10)	.	.	no
H7	H8	2.235(11)	.	.	no
H7	C17	2.79(2)	.	.	no
H7	H17	2.21(3)	.	.	no
H7'	H6"	2.355(19)	.	.	no
H7'	C16	3.060(15)	.	.	no
H7'	H17	2.54(3)	.	.	no
H7'	C6	2.972(11)	.	.	no
H7'	H16	2.35(3)	.	.	no
H7"	F2	2.584(19)	.	2_666	no
H8	H17'	2.16(3)	.	.	no
H8	C17	2.943(17)	.	.	no
H8	H7	2.235(11)	.	.	no
H8	C7	2.869(7)	.	.	no
H8"	H18"	2.50(3)	.	.	no
H8"	C18	3.09(2)	.	.	no
H8"	H9	2.53(2)	.	.	no
H8"	C9	2.885(11)	.	.	no
H9	C8	3.065(18)	.	.	no
H9	H8"	2.53(2)	.	.	no
H9'	C28	2.823(19)	.	.	no
H9'	C44	3.095(15)	.	.	no
H9'	C29	3.09(2)	.	.	no
H9'	C27	2.857(17)	.	.	no
H9'	H44	2.283(14)	.	.	no
H9"	H26	2.528(17)	.	.	no
H9"	C10	2.836(6)	.	.	no
H9"	H10"	2.213(12)	.	.	no
H10	C24	2.900(13)	.	2_565	no
H10	C23	3.053(11)	.	2_565	no
H10'	F1	2.668(14)	.	.	no
H10'	H6	2.46(2)	.	.	no
H10'	C21	2.923(15)	.	.	no
H10'	C6	2.939(16)	.	.	no
H10"	C21	2.82(2)	.	.	no
H10"	C9	2.862(11)	.	.	no
H10"	H9"	2.213(12)	.	.	no
H10"	C26	2.953(19)	.	.	no
H10"	F1	2.79(2)	.	.	no
H16	C17	2.834(14)	.	.	no
H16	H7'	2.35(3)	.	.	no
H16	H17	2.245(17)	.	.	no
H16'	H41	2.56(2)	.	1_545	no
H16"	C54	3.089(13)	.	1_455	no

H16"	C20	2.968(15)	.	.	no
H16"	H20'	2.49(2)	.	.	no
H17	H7'	2.54(3)	.	.	no
H17	H7	2.21(3)	.	.	no
H17	C16	2.867(12)	.	.	no
H17	C7	2.73(2)	.	.	no
H17	H16	2.245(17)	.	.	no
H17	H34	2.568(11)	.	2_666	no
H17'	H18"	2.274(16)	.	.	no
H17'	H8	2.16(3)	.	.	no
H17'	C42	2.946(10)	.	2_666	no
H17'	C8	2.92(2)	.	.	no
H17'	C18	2.900(10)	.	.	no
H17"	H17"	2.558(11)	.	2_656	no
H18	C19	2.978(17)	.	.	no
H18	H19"	2.44(2)	.	.	no
H18	C49	3.094(14)	.	2_665	no
H18'	C35	3.016(16)	.	1_545	no
H18'	C34	2.902(11)	.	1_545	no
H18"	C17	2.805(13)	.	.	no
H18"	H17'	2.274(16)	.	.	no
H18"	H8"	2.50(3)	.	.	no
H18"	C8	3.09(2)	.	.	no
H19	C21	2.90(2)	.	.	no
H19	H20	2.224(13)	.	.	no
H19	Ti1	3.605(18)	.	.	no
H19	F1	2.63(2)	.	.	no
H19	C20	2.860(8)	.	.	no
H19'	C50	2.73(2)	.	1_545	no
H19'	C49	3.012(17)	.	1_545	no
H19"	C18	2.904(14)	.	.	no
H19"	H18	2.44(2)	.	.	no
H19"	Ti1	3.487(18)	.	.	no
H20	F1	2.82(2)	.	.	no
H20	C19	2.830(12)	.	.	no
H20	H19	2.224(13)	.	.	no
H20	Ti1	3.66(2)	.	.	no
H20'	Ti1	3.431(14)	.	.	no
H20'	C16	2.96(2)	.	.	no
H20'	H16"	2.49(2)	.	.	no
H20"	H37	2.588(13)	.	1_445	no
H22	C47	2.738(4)	.	2_565	no
H23	C43	3.003(4)	.	2_565	no
H23	C39	3.026(4)	.	2_565	no
H23	C44	3.074(4)	.	2_565	no
H23	C41	2.747(4)	.	2_565	no
H23	C40	2.801(4)	.	2_565	no
H23	C42	2.872(4)	.	2_565	no
H24	C56	2.840(4)	.	1_454	no
H24	C42	2.889(4)	.	2_565	no
H24	C55	3.099(4)	.	1_454	no
H25	C31	3.007(4)	.	2_665	no
H25	C32	3.090(4)	.	2_665	no
H25	C30	3.037(4)	.	2_665	no
H26	C28	2.989(4)	.	2_665	no
H26	H9"	2.528(17)	.	.	no
H28	C45	2.637(3)	.	.	no
H28	C46	2.712(4)	.	.	no
H30	C47	3.038(4)	.	2_665	no
H31	F2	2.474(4)	.	.	no
H31	C52	3.067(4)	.	.	no
H31	H56	2.506(4)	.	2_766	no
H31	H51	2.47(11)	.	.	no
H31	H52	2.482(4)	.	.	no
H32	C39	2.967(4)	.	.	no
H32	C44	2.952(4)	.	.	no

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 H32     C33        3.001(3)                    .       .                 no
 H32     C7         2.876(4)                    .     2_666               no
 H34     C39        2.667(3)                    .       .                 no
 H34     C40        2.585(4)                    .       .                 no
 H34     H40        2.498(4)                    .       .                 no
 H34     H17       2.568(11)                    .     2_666               no
 H35     F21        2.633(7)                    .     1_565               no
 H35     H53        2.529(4)                    .     1_565               no
 H36     F21        2.776(6)                    .     1_565               no
 H37     H20"      2.588(13)                    .     1_665               no
 H38     C27        2.983(3)                    .       .                 no
 H38     C26        2.937(4)                    .     2_665               no
 H38     H50        2.448(4)                    .       .                 no
 H38     C45        3.006(4)                    .       .                 no
 H38     C50        2.894(4)                    .       .                 no
 H40     C34        2.917(4)                    .       .                 no
 H40     C33        2.961(4)                    .       .                 no
 H40     H34        2.498(4)                    .       .                 no
 H40     C14        3.011(4)                    .     1_565               no
 H40     C13        3.080(4)                    .     1_565               no
 H41     C11        2.823(4)                    .     1_565               no
 H41     H16'        2.56(2)                    .     1_565               no
 H42     C52        2.972(4)                    .     2_666               no
 H42     C53        2.971(4)                    .     2_666               no
 H44     C27        2.721(4)                    .       .                 no
 H44     C32        2.684(4)                    .       .                 no
 H44     C9         3.055(4)                    .       .                 no
 H44     H9'       2.283(14)                    .       .                 no
 H46     C39        2.929(3)                    .       .                 no
 H46     C27        3.048(4)                    .       .                 no
 H49     C37        2.874(4)                    .     2_675               no
 H49     C38        3.055(4)                    .     2_675               no
 H50     H38        2.448(4)                    .       .                 no
 H50     C33        2.751(3)                    .       .                 no
 H50     C38        2.653(4)                    .       .                 no
 H51     H31        2.47(11)                    .       .                 no
 H52     C31        3.093(4)                    .       .                 no
 H52     H31        2.482(4)                    .       .                 no
 H53     H35        2.529(4)                    .     1_545               no
 H53     C36        3.001(4)                    .     1_545               no
 H53     C35        2.932(4)                    .     1_545               no
 H54     C16         3.01(7)                    .     1_655               no
 H55     C35        2.869(4)                    .     2_766               no
 H55     C36        2.924(4)                    .     2_766               no
 H56     H31        2.506(4)                    .     2_766               no
 H56     C31        2.857(4)                    .     2_766               no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C31     H31     F2        0.950(4)   2.474(4)   3.422(4)   175.8(3)     .   yes

#===END of Crystallographic Information File
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