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Versatile coordination of cyclopentadienyl-arene ligands and its role in titanium-catalyzed ethylene trimerization

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_audit_update_record
;
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;

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

_publ_contact_letter                 # Include date of submission
;
  Date of submission :  2007-11-07  13:56:53

  Consider this CIF submission for deposition of the fourth
  X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : Q1127)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_to_coeditor            ?

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_journal_date_accepted           ?

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_journal_date_printers_final     ?
_journal_date_proofs_out         ?
_journal_date_proofs_in          ?

_journal_coeditor_name           ?
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_journal_page_last               ?

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3. TITLE AND AUTHOR LIST

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_publ_section_title
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?
;
_publ_section_title_footnote
;
?
;

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```

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

```

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loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
; # author related footnote
;
; # Address of this author
;
'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

_publ_section_synopsis
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?
;
_publ_section_abstract
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?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
;
_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 displacement parameters for
the non-hydrogen atoms were refined. A subsequent difference Fourier synthesis
resulted in the location of all the hydrogen atoms, which coordinates and
isotropic displacement parameters were refined.
Refinement was frustrated by a disorder problem: from the solution it was clear
that the positions of a solvate molecule were highly disordered.
No satisfactory discrete model could be fitted in this density.
The BYPASS (SQUEEZE) procedure was used to take into account the electron
density in the potential solvent area (348.5 Å3/unit cell).
;

# Insert blank lines between references

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

Beurskens, P.T., Beurskens, G., Gelder, R. de, Garcia-Granda, S.
Gould, R.O., Israel, & Smits, J.M.M. (1999).
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Laboratory, University of Nijmegen, The Netherlands.

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```

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Wilson, A.J.C. (1992). Ed. International Tables for Crystallography, Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.

;

_publ_section_figure_captions

;

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.

;

#=====

5. CHEMICAL DATA

_chemical_name_systematic

;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C₂₉ H₄₀ N₂ V, C₂₄ B F₂₀'

Ex: 'C₁₂ H₁₆ N₂ O₆, H₂ O' and '(Cd²⁺)₃, (C₆ N₆ Cr³⁻)₂, 2(H₂ O)'

_chemical_formula_structural ?

_chemical_formula_sum

'C₅₃ H₄₀ B F₂₀ N₂ V'

_chemical_formula_iupac ?

_chemical_formula_weight 1146.63

_chemical_compound_source 'see text'

```

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
V    V    0.3005    0.5294
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N    N    0.0061    0.0033
'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'
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 2yn'
_symmetry_space_group_name_H-M 'P 21/n'
_symmetry_Int_Tables_number 14

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,1/2-z
3 -x,-y,-z
4 1/2+x,1/2-y,1/2+z

_cell_length_a      15.858(2)
_cell_length_b      15.996(2)
_cell_length_c      20.876(2)
_cell_angle_alpha    90
_cell_angle_beta     104.360(2)
_cell_angle_gamma     90
_cell_volume         5130.1(10)
_cell_formula_units_Z 4

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 5280
_cell_measurement_theta_min 2.25
_cell_measurement_theta_max 28.30
_cell_special_details

;
The final unit cell was obtained from the xyz centroids of
5280 reflections after integration using the SAINTPLUS
software package (Bruker, 2000).

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          'red'
_exptl_crystal_size_max        0.47
_exptl_crystal_size_mid        0.28
_exptl_crystal_size_min        0.19
_exptl_crystal_size_rad        ?
_exptl_crystal_density_meas    ?
_exptl_crystal_density_diffn   1.485
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           2320
_exptl_absorpt_coefficient_mu   0.305
_exptl_absorpt_correction_type  'Multi-Scan'
_exptl_absorpt_process_details  '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min 0.8465
_exptl_absorpt_correction_T_max 0.9437

```

```

#=====

```

``` # 7. EXPERIMENTAL DATA ```

```

_exptl_special_details
;
;
_diffn_ambient_temperature      100(1)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           'MoK\alpha'
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator  'parallel mounted graphite'
_diffn_radiation_detector
;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean  66.06

_diffn_standards_number          0
_diffn_standards_interval_count  ?
_diffn_standards_interval_time   ?
_diffn_standards_decay_%         0

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number            41370
_diffn_reflns_av_R_equivalents  0.0437
_diffn_reflns_av_sigmaI/netI    0.0450
_diffn_reflns_limit_h_min       -20
_diffn_reflns_limit_h_max       20

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```

_diffrn_reflms_limit_k_min      -20
_diffrn_reflms_limit_k_max      20
_diffrn_reflms_limit_l_min      -25
_diffrn_reflms_limit_l_max      26
_diffrn_reflms_theta_min        2.47
_diffrn_reflms_theta_max        26.73
_diffrn_measured_fraction_theta_max 0.996
_diffrn_reflms_theta_full       25.00
_diffrn_measured_fraction_theta_full 0.998

_diffrn_reflms_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflms_number_total            10849
_reflms_number_gt               8324
_reflms_threshold_expression     $I > 2\sigma(I)$ 

_computing_data_collection      'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement      'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction       'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2006)
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
 $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on  $F^2$  are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\sigma^2(Fo^2)+(0.0588P)^2+0.9039P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary     heavy
_atom_sites_solution_secondary   direct

```


_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	10849
_refine_ls_number_parameters	854
_refine_ls_number_restraints	0
_refine_ls_number_constraints	?
_refine_ls_R_factor_all	0.0597
_refine_ls_R_factor_gt	0.0432
_refine_ls_wR_factor_ref	0.1106
_refine_ls_wR_factor_gt	0.1041
_refine_ls_goodness_of_fit_ref	1.026
_refine_ls_restrained_S_all	1.026
_refine_ls_shift/su_max	0.001
_refine_ls_shift/su_mean	0.000
_refine_diff_density_max	0.418
_refine_diff_density_min	-0.318
_refine_diff_density_rms	0.060
_vrn_publ_code_void_volume	348.5
_vrn_publ_code_frame_time_sec	10.0
_vrn_publ_code_meas_time_hour	10.5

#=====

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_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
V1 V Uani 0.02372(2) 0.10185(2) 0.18943(2) 1.000 0.0164(1) . .
N11 N Uani 0.06965(10) 0.10200(10) 0.12519(8) 1.000 0.0188(5) . .
N12 N Uani -0.09581(10) 0.09926(10) 0.15012(8) 1.000 0.0190(5) . .
C11 C Uani 0.01395(14) 0.17336(13) 0.28434(11) 1.000 0.0248(6) . .
C12 C Uani 0.02346(15) 0.23067(13) 0.23492(11) 1.000 0.0269(7) . .
C13 C Uani 0.10620(15) 0.21810(13) 0.22312(11) 1.000 0.0269(7) . .
C14 C Uani 0.14669(14) 0.15219(14) 0.26293(11) 1.000 0.0256(7) . .
C15 C Uani 0.08976(13) 0.12386(13) 0.30126(10) 1.000 0.0222(6) . .
C16 C Uani 0.09944(13) 0.04453(14) 0.34234(11) 1.000 0.0258(6) . .
C17 C Uani 0.19486(15) 0.01598(17) 0.36358(14) 1.000 0.0359(8) . .
C18 C Uani 0.06660(16) 0.05892(17) 0.40441(12) 1.000 0.0325(8) . .
C19 C Uani 0.04429(13) -0.01860(12) 0.29445(10) 1.000 0.0217(6) . .
C110 C Uani -0.02895(13) -0.05764(13) 0.30546(11) 1.000 0.0228(6) . .
C111 C Uani -0.07813(13) -0.11366(12) 0.26008(11) 1.000 0.0238(6) . .
C112 C Uani -0.05350(14) -0.13091(13) 0.20237(12) 1.000 0.0254(7) . .
C113 C Uani 0.01873(13) -0.09329(12) 0.18823(11) 1.000 0.0231(6) . .
C114 C Uani 0.06626(13) -0.03524(12) 0.23389(11) 1.000 0.0218(6) . .
C115 C Uani -0.15721(17) -0.15395(15) 0.27458(15) 1.000 0.0317(8) . .

```

C116 C Uani 0.04875(17) -0.11742(15) 0.12794(13) 1.000 0.0316(8) . .
 C117 C Uani 0.13017(12) 0.12106(12) 0.08926(10) 1.000 0.0184(6) . .
 C118 C Uani 0.11253(15) 0.17980(14) 0.03833(12) 1.000 0.0303(7) . .
 C119 C Uani 0.17379(15) 0.19621(15) 0.00293(12) 1.000 0.0315(7) . .
 C120 C Uani 0.25357(14) 0.15589(13) 0.01675(11) 1.000 0.0262(7) . .
 C121 C Uani 0.27117(14) 0.09904(14) 0.06852(11) 1.000 0.0268(7) . .
 C122 C Uani 0.21083(13) 0.08116(13) 0.10436(11) 1.000 0.0228(6) . .
 C123 C Uani 0.31814(18) 0.17303(18) -0.02391(14) 1.000 0.0380(9) . .
 C124 C Uani -0.15985(13) 0.09461(13) 0.19166(12) 1.000 0.0251(7) . .
 C125 C Uani -0.20684(16) 0.17810(16) 0.19339(14) 1.000 0.0325(8) . .
 C126 C Uani -0.22543(16) 0.02382(16) 0.16932(16) 1.000 0.0340(8) . .
 C127 C Uani -0.13919(13) 0.11158(13) 0.07910(11) 1.000 0.0242(6) . .
 C128 C Uani -0.12313(16) 0.20005(15) 0.05692(13) 1.000 0.0300(7) . .
 C129 C Uani -0.11305(17) 0.04484(17) 0.03591(13) 1.000 0.0363(8) . .

H11 H Uiso -0.0346(14) 0.1661(13) 0.3009(10) 1.000 0.018(5) . .
 H12 H Uiso -0.0186(14) 0.2676(14) 0.2140(11) 1.000 0.023(6) . .
 H13 H Uiso 0.1279(14) 0.2490(14) 0.1911(11) 1.000 0.025(6) . .
 H14 H Uiso 0.2001(16) 0.1276(15) 0.2616(12) 1.000 0.033(6) . .
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 H17" H Uiso 0.2298(17) 0.0620(16) 0.3930(13) 1.000 0.041(7) . .
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 H18' H Uiso 0.0718(15) 0.0073(16) 0.4315(12) 1.000 0.034(6) . .
 H18" H Uiso 0.0048(16) 0.0841(14) 0.3909(11) 1.000 0.026(6) . .
 H110 H Uiso -0.0461(14) -0.0488(13) 0.3439(11) 1.000 0.019(5) . .
 H112 H Uiso -0.0867(16) -0.1655(15) 0.1709(12) 1.000 0.034(7) . .
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 H115 H Uiso -0.187(2) -0.189(2) 0.2393(17) 1.000 0.070(10) . .
 H115' H Uiso -0.195(2) -0.115(2) 0.2792(16) 1.000 0.070(10) . .
 H115" H Uiso -0.142(2) -0.188(2) 0.3091(19) 1.000 0.081(12) . .
 H116 H Uiso 0.0825(19) -0.169(2) 0.1367(15) 1.000 0.064(9) . .
 H116' H Uiso 0.0832(19) -0.075(2) 0.1112(15) 1.000 0.062(9) . .
 H116" H Uiso -0.001(2) -0.135(2) 0.0950(19) 1.000 0.085(12) . .
 H118 H Uiso 0.0583(17) 0.2073(16) 0.0323(12) 1.000 0.039(7) . .
 H119 H Uiso 0.1609(18) 0.2407(18) -0.0300(14) 1.000 0.053(8) . .
 H121 H Uiso 0.3233(18) 0.0718(17) 0.0785(13) 1.000 0.045(7) . .
 H122 H Uiso 0.2214(14) 0.0395(14) 0.1393(12) 1.000 0.030(6) . .
 H123 H Uiso 0.336(2) 0.233(3) -0.0190(19) 1.000 0.091(12) . .
 H123' H Uiso 0.286(3) 0.174(3) -0.073(3) 1.000 0.139(18) . .
 H123" H Uiso 0.373(3) 0.153(3) 0.000(2) 1.000 0.106(14) . .
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 H127 H Uiso -0.2012(14) 0.1065(13) 0.0759(10) 1.000 0.020(5) . .
 H128 H Uiso -0.1460(17) 0.2430(18) 0.0844(14) 1.000 0.050(8) . .
 H128' H Uiso -0.1537(16) 0.2053(16) 0.0133(14) 1.000 0.038(7) . .
 H128" H Uiso -0.0567(17) 0.2065(16) 0.0650(12) 1.000 0.041(7) . .
 H129 H Uiso -0.0533(17) 0.0453(15) 0.0365(12) 1.000 0.036(7) . .
 H129' H Uiso -0.1484(17) 0.0542(16) -0.0090(14) 1.000 0.044(7) . .
 H129" H Uiso -0.1249(18) -0.0160(18) 0.0567(14) 1.000 0.055(8) . .

F22 F Uani 0.64559(7) 0.17605(7) 0.30190(6) 1.000 0.0250(4) . .
 F23 F Uani 0.80970(8) 0.16014(8) 0.36912(6) 1.000 0.0326(4) . .
 F24 F Uani 0.86974(7) 0.01233(8) 0.42824(6) 1.000 0.0315(4) . .

F25 F Uani 0.76119(8) -0.12246(8) 0.41282(6) 1.000 0.0294(4) . .
 F26 F Uani 0.59790(7) -0.10993(7) 0.34169(6) 1.000 0.0231(4) . .
 F28 F Uani 0.35520(7) 0.15876(7) 0.28068(6) 1.000 0.0286(4) . .
 F29 F Uani 0.30458(8) 0.28262(8) 0.19748(7) 1.000 0.0387(4) . .
 F210 F Uani 0.38932(9) 0.31815(8) 0.10194(7) 1.000 0.0395(5) . .
 F211 F Uani 0.53108(9) 0.22483(8) 0.09486(6) 1.000 0.0358(4) . .
 F212 F Uani 0.58366(7) 0.09849(7) 0.17824(6) 1.000 0.0256(4) . .
 F214 F Uani 0.32690(7) -0.01407(7) 0.23217(6) 1.000 0.0245(4) . .
 F215 F Uani 0.26153(8) -0.12743(8) 0.13971(7) 1.000 0.0359(4) . .
 F216 F Uani 0.36765(9) -0.21421(9) 0.07905(7) 1.000 0.0418(5) . .
 F217 F Uani 0.54253(9) -0.18530(8) 0.11510(6) 1.000 0.0347(4) . .
 F218 F Uani 0.61019(7) -0.07617(7) 0.20810(6) 1.000 0.0252(4) . .
 F220 F Uani 0.51566(8) 0.16951(7) 0.37562(6) 1.000 0.0277(4) . .
 F221 F Uani 0.45507(8) 0.17041(8) 0.48352(7) 1.000 0.0375(4) . .
 F222 F Uani 0.37484(8) 0.03261(9) 0.51770(6) 1.000 0.0368(4) . .
 F223 F Uani 0.36059(8) -0.10782(8) 0.44201(6) 1.000 0.0307(4) . .
 F224 F Uani 0.41830(7) -0.11037(7) 0.33420(6) 1.000 0.0231(3) . .
 C21 C Uani 0.61244(12) 0.03283(12) 0.31557(9) 1.000 0.0175(6) . .
 C22 C Uani 0.67060(13) 0.09887(12) 0.32636(10) 1.000 0.0207(6) . .
 C23 C Uani 0.75656(13) 0.09309(13) 0.36235(10) 1.000 0.0228(6) . .
 C24 C Uani 0.78732(12) 0.01883(13) 0.39195(10) 1.000 0.0232(6) . .
 C25 C Uani 0.73257(13) -0.04939(12) 0.38397(10) 1.000 0.0207(6) . .
 C26 C Uani 0.64809(12) -0.04080(12) 0.34634(10) 1.000 0.0198(6) . .
 C27 C Uani 0.47420(12) 0.12175(12) 0.23562(10) 1.000 0.0199(6) . .
 C28 C Uani 0.40315(13) 0.17213(12) 0.23635(10) 1.000 0.0229(6) . .
 C29 C Uani 0.37432(14) 0.23736(13) 0.19304(11) 1.000 0.0277(7) . .
 C210 C Uani 0.41696(15) 0.25547(12) 0.14518(11) 1.000 0.0283(7) . .
 C211 C Uani 0.48798(14) 0.20793(13) 0.14125(11) 1.000 0.0270(7) . .
 C212 C Uani 0.51389(13) 0.14342(12) 0.18565(10) 1.000 0.0222(6) . .
 C213 C Uani 0.47225(12) -0.03853(11) 0.22612(10) 1.000 0.0179(6) . .
 C214 C Uani 0.38419(13) -0.05595(12) 0.20467(10) 1.000 0.0200(6) . .
 C215 C Uani 0.34812(13) -0.11326(13) 0.15669(11) 1.000 0.0255(6) . .
 C216 C Uani 0.40090(15) -0.15718(13) 0.12564(10) 1.000 0.0273(7) . .
 C217 C Uani 0.48933(14) -0.14250(13) 0.14419(10) 1.000 0.0254(7) . .
 C218 C Uani 0.52234(13) -0.08466(12) 0.19306(10) 1.000 0.0207(6) . .
 C219 C Uani 0.46624(12) 0.03152(12) 0.34631(10) 1.000 0.0181(6) . .
 C220 C Uani 0.47566(12) 0.09921(12) 0.38936(10) 1.000 0.0216(6) . .
 C221 C Uani 0.44507(13) 0.10130(13) 0.44561(11) 1.000 0.0253(6) . .
 C222 C Uani 0.40539(13) 0.03210(15) 0.46302(10) 1.000 0.0261(7) . .
 C223 C Uani 0.39794(13) -0.03856(13) 0.42476(10) 1.000 0.0227(6) . .
 C224 C Uani 0.42853(12) -0.03779(12) 0.36845(10) 1.000 0.0189(6) . .
 B2 B Uani 0.50679(14) 0.03690(14) 0.28100(11) 1.000 0.0184(6) . .

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
 V1 0.0156(2) 0.0164(2) 0.0188(2) 0.0013(1) 0.0070(1) 0.0010(1)
 N11 0.0176(8) 0.0173(8) 0.0227(9) -0.0001(7) 0.0074(7) 0.0002(6)
 N12 0.0186(8) 0.0163(8) 0.0247(9) 0.0017(7) 0.0102(7) 0.0008(6)
 C11 0.0265(11) 0.0255(11) 0.0241(11) -0.0039(9) 0.0093(9) 0.0010(9)
 C12 0.0364(12) 0.0189(10) 0.0250(12) -0.0014(9) 0.0071(10) 0.0026(9)
 C13 0.0365(12) 0.0199(10) 0.0259(12) -0.0025(9) 0.0108(10) -0.0078(9)
 C14 0.0243(11) 0.0267(11) 0.0255(12) -0.0016(9) 0.0059(9) -0.0065(9)
 C15 0.0213(10) 0.0242(10) 0.0204(11) -0.0019(8) 0.0040(8) -0.0043(8)
 C16 0.0206(10) 0.0327(12) 0.0231(11) 0.0054(9) 0.0038(9) -0.0023(9)

C17 0.0214(11) 0.0438(15) 0.0372(15) 0.0127(12) -0.0029(10) -0.0003(10)
C18 0.0345(13) 0.0412(14) 0.0209(12) 0.0046(10) 0.0050(10) -0.0081(11)
C19 0.0184(10) 0.0203(10) 0.0262(11) 0.0086(8) 0.0049(8) 0.0062(8)
C110 0.0240(10) 0.0219(10) 0.0260(12) 0.0079(9) 0.0131(9) 0.0045(8)
C111 0.0235(10) 0.0142(10) 0.0371(13) 0.0050(9) 0.0141(9) 0.0035(8)
C112 0.0241(11) 0.0164(10) 0.0385(14) -0.0023(9) 0.0129(10) -0.0003(8)
C113 0.0229(10) 0.0171(10) 0.0317(12) 0.0042(8) 0.0116(9) 0.0050(8)
C114 0.0170(10) 0.0205(10) 0.0308(12) 0.0083(9) 0.0117(9) 0.0033(8)
C115 0.0300(12) 0.0199(11) 0.0532(17) -0.0033(11) 0.0254(12) -0.0056(10)
C116 0.0338(13) 0.0267(12) 0.0407(15) -0.0045(10) 0.0215(12) -0.0012(10)
C117 0.0199(10) 0.0184(10) 0.0187(10) -0.0023(8) 0.0084(8) -0.0017(8)
C118 0.0290(12) 0.0317(12) 0.0346(13) 0.0102(10) 0.0162(10) 0.0091(10)
C119 0.0371(13) 0.0297(12) 0.0324(13) 0.0106(10) 0.0176(11) 0.0027(10)
C120 0.0267(11) 0.0280(11) 0.0275(12) -0.0017(9) 0.0137(9) -0.0056(9)
C121 0.0177(10) 0.0362(12) 0.0274(12) 0.0022(10) 0.0076(9) 0.0015(9)
C122 0.0199(10) 0.0281(11) 0.0203(11) 0.0021(9) 0.0048(8) -0.0002(8)
C123 0.0331(14) 0.0488(16) 0.0382(16) 0.0070(12) 0.0204(12) -0.0043(12)
C124 0.0181(10) 0.0274(11) 0.0337(13) 0.0087(9) 0.0138(9) 0.0056(8)
C125 0.0283(12) 0.0331(13) 0.0426(16) 0.0055(11) 0.0214(12) 0.0085(10)
C126 0.0210(11) 0.0317(14) 0.0526(17) 0.0143(12) 0.0152(12) 0.0018(10)
C127 0.0164(10) 0.0278(11) 0.0273(12) 0.0004(9) 0.0031(9) -0.0029(8)
C128 0.0268(12) 0.0364(13) 0.0249(13) 0.0123(10) 0.0026(10) 0.0014(10)
C129 0.0308(13) 0.0450(15) 0.0311(14) -0.0138(11) 0.0040(11) -0.0023(11)
F22 0.0245(6) 0.0193(6) 0.0310(7) 0.0007(5) 0.0065(5) -0.0036(5)
F23 0.0262(6) 0.0346(7) 0.0362(8) -0.0034(6) 0.0063(6) -0.0135(5)
F24 0.0175(6) 0.0470(8) 0.0272(7) 0.0011(6) 0.0001(5) -0.0016(5)
F25 0.0248(6) 0.0318(7) 0.0306(7) 0.0088(5) 0.0048(5) 0.0063(5)
F26 0.0212(6) 0.0196(6) 0.0277(7) 0.0024(5) 0.0048(5) -0.0016(4)
F28 0.0213(6) 0.0299(7) 0.0365(7) 0.0022(5) 0.0109(5) 0.0042(5)
F29 0.0328(7) 0.0297(7) 0.0496(9) 0.0028(6) 0.0028(6) 0.0125(6)
F210 0.0526(9) 0.0244(7) 0.0344(8) 0.0097(6) -0.0024(6) 0.0014(6)
F211 0.0476(8) 0.0352(7) 0.0258(7) 0.0077(6) 0.0116(6) -0.0084(6)
F212 0.0251(6) 0.0302(6) 0.0238(7) 0.0029(5) 0.0103(5) 0.0014(5)
F214 0.0180(6) 0.0291(6) 0.0259(7) -0.0019(5) 0.0046(5) 0.0033(5)
F215 0.0227(6) 0.0370(7) 0.0415(8) -0.0086(6) -0.0043(6) -0.0047(5)
F216 0.0468(8) 0.0391(8) 0.0343(8) -0.0187(6) 0.0003(7) -0.0065(6)
F217 0.0428(8) 0.0354(7) 0.0312(7) -0.0123(6) 0.0191(6) -0.0008(6)
F218 0.0216(6) 0.0292(6) 0.0284(7) -0.0055(5) 0.0128(5) -0.0025(5)
F220 0.0283(6) 0.0225(6) 0.0338(7) -0.0083(5) 0.0104(5) -0.0040(5)
F221 0.0354(7) 0.0432(8) 0.0350(8) -0.0220(6) 0.0107(6) 0.0015(6)
F222 0.0328(7) 0.0607(9) 0.0209(7) -0.0014(6) 0.0142(6) 0.0073(6)
F223 0.0287(7) 0.0382(7) 0.0285(7) 0.0106(6) 0.0136(5) -0.0008(5)
F224 0.0277(6) 0.0192(6) 0.0244(6) -0.0013(5) 0.0103(5) -0.0032(5)
C21 0.0180(9) 0.0206(10) 0.0162(10) -0.0032(8) 0.0087(8) -0.0012(8)
C22 0.0237(10) 0.0206(10) 0.0197(10) -0.0022(8) 0.0089(8) -0.0005(8)
C23 0.0208(10) 0.0275(11) 0.0217(11) -0.0060(8) 0.0083(8) -0.0099(8)
C24 0.0143(9) 0.0364(12) 0.0192(11) -0.0035(9) 0.0046(8) 0.0002(8)
C25 0.0219(10) 0.0239(10) 0.0180(10) 0.0024(8) 0.0083(8) 0.0056(8)
C26 0.0204(10) 0.0220(10) 0.0199(10) -0.0036(8) 0.0103(8) -0.0038(8)
C27 0.0185(10) 0.0174(9) 0.0227(11) -0.0017(8) 0.0032(8) -0.0040(7)
C28 0.0220(10) 0.0213(10) 0.0248(11) -0.0007(8) 0.0047(9) -0.0025(8)
C29 0.0251(11) 0.0183(10) 0.0352(13) -0.0019(9) -0.0010(10) 0.0029(8)
C210 0.0355(12) 0.0163(10) 0.0271(12) 0.0036(9) -0.0037(10) -0.0023(9)
C211 0.0324(12) 0.0251(11) 0.0226(12) 0.0008(9) 0.0049(9) -0.0101(9)
C212 0.0204(10) 0.0223(10) 0.0222(11) -0.0002(8) 0.0021(8) -0.0017(8)
C213 0.0205(10) 0.0165(9) 0.0168(10) 0.0023(8) 0.0050(8) -0.0002(8)
C214 0.0223(10) 0.0202(10) 0.0178(10) 0.0025(8) 0.0054(8) 0.0029(8)
C215 0.0218(10) 0.0257(11) 0.0248(12) 0.0020(9) -0.0019(9) -0.0015(8)
C216 0.0357(12) 0.0236(11) 0.0203(11) -0.0056(9) 0.0024(9) -0.0053(9)
C217 0.0333(12) 0.0238(11) 0.0216(11) -0.0011(9) 0.0116(9) -0.0002(9)
C218 0.0217(10) 0.0216(10) 0.0199(10) 0.0018(8) 0.0075(8) -0.0027(8)

```

C219 0.0135(9) 0.0214(10) 0.0193(10) -0.0008(8) 0.0038(8) 0.0037(7)
C220 0.0162(9) 0.0211(10) 0.0271(11) -0.0022(8) 0.0046(8) -0.0002(8)
C221 0.0203(10) 0.0318(12) 0.0228(11) -0.0110(9) 0.0034(9) 0.0057(9)
C222 0.0168(10) 0.0482(14) 0.0139(10) -0.0023(9) 0.0052(8) 0.0065(9)
C223 0.0168(9) 0.0307(11) 0.0211(11) 0.0062(9) 0.0056(8) 0.0028(8)
C224 0.0175(9) 0.0200(10) 0.0193(10) -0.0002(8) 0.0047(8) 0.0023(8)
B2 0.0180(10) 0.0178(11) 0.0209(12) 0.0000(9) 0.0076(9) 0.0008(8)

```

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

``` # 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
```

V1	N11	1.6774(17)	.	.	yes
V1	N12	1.8699(17)	.	.	yes
V1	C11	2.326(2)	.	.	yes
V1	C12	2.269(2)	.	.	yes
V1	C13	2.282(2)	.	.	yes
V1	C14	2.307(2)	.	.	yes
V1	C15	2.336(2)	.	.	yes
V1	C114	2.411(2)	.	.	yes
F22	C22	1.357(2)	.	.	yes
F23	C23	1.350(2)	.	.	yes
F24	C24	1.342(2)	.	.	yes
F25	C25	1.341(2)	.	.	yes
F26	C26	1.352(2)	.	.	yes
F28	C28	1.353(2)	.	.	yes
F29	C29	1.344(3)	.	.	yes
F210	C210	1.348(2)	.	.	yes
F211	C211	1.344(3)	.	.	yes
F212	C212	1.360(2)	.	.	yes
F214	C214	1.365(2)	.	.	yes
F215	C215	1.350(3)	.	.	yes
F216	C216	1.342(3)	.	.	yes
F217	C217	1.343(3)	.	.	yes
F218	C218	1.357(2)	.	.	yes
F220	C220	1.356(2)	.	.	yes
F221	C221	1.346(3)	.	.	yes
F222	C222	1.346(2)	.	.	yes
F223	C223	1.347(2)	.	.	yes
F224	C224	1.352(2)	.	.	yes
N11	C117	1.391(3)	.	.	yes
N12	C127	1.485(3)	.	.	yes
N12	C124	1.492(3)	.	.	yes
C11	C12	1.416(3)	.	.	no
C11	C15	1.409(3)	.	.	no

C12	C13	1.408(3)	.	.	no
C13	C14	1.396(3)	.	.	no
C14	C15	1.421(3)	.	.	no
C15	C16	1.518(3)	.	.	no
C16	C19	1.533(3)	.	.	no
C16	C18	1.529(3)	.	.	no
C16	C17	1.537(3)	.	.	no
C19	C110	1.387(3)	.	.	no
C19	C114	1.417(3)	.	.	no
C110	C111	1.394(3)	.	.	no
C11	H11	0.93(2)	.	.	no
C111	C115	1.506(3)	.	.	no
C111	C112	1.383(3)	.	.	no
C112	C113	1.389(3)	.	.	no
C12	H12	0.92(2)	.	.	no
C113	C114	1.408(3)	.	.	no
C113	C116	1.502(3)	.	.	no
C13	H13	0.96(2)	.	.	no
C14	H14	0.94(3)	.	.	no
C17	H17"	1.03(3)	.	.	no
C117	C122	1.394(3)	.	.	no
C17	H17	1.03(3)	.	.	no
C17	H17'	0.99(3)	.	.	no
C117	C118	1.394(3)	.	.	no
C18	H18'	0.99(3)	.	.	no
C18	H18	1.01(3)	.	.	no
C118	C119	1.384(3)	.	.	no
C18	H18"	1.03(3)	.	.	no
C119	C120	1.385(3)	.	.	no
C120	C121	1.387(3)	.	.	no
C120	C123	1.508(4)	.	.	no
C121	C122	1.383(3)	.	.	no
C124	C125	1.534(3)	.	.	no
C124	C126	1.530(3)	.	.	no
C127	C128	1.530(3)	.	.	no
C127	C129	1.520(3)	.	.	no
C110	H110	0.92(2)	.	.	no
C112	H112	0.92(2)	.	.	no
C114	H114	0.94(3)	.	.	no
C115	H115"	0.89(4)	.	.	no
C115	H115	0.95(3)	.	.	no
C115	H115'	0.89(3)	.	.	no
C116	H116'	0.99(3)	.	.	no
C116	H116"	0.95(4)	.	.	no
C116	H116	0.98(3)	.	.	no
C118	H118	0.95(3)	.	.	no
C119	H119	0.98(3)	.	.	no
C21	C26	1.393(3)	.	.	no
C21	B2	1.653(3)	.	.	yes
C121	H121	0.91(3)	.	.	no
C21	C22	1.384(3)	.	.	no
C122	H122	0.97(2)	.	.	no
C22	C23	1.387(3)	.	.	no
C123	H123'	1.03(6)	.	.	no
C23	C24	1.372(3)	.	.	no
C123	H123	1.00(5)	.	.	no
C123	H123"	0.95(5)	.	.	no
C124	H124	1.01(2)	.	.	no
C24	C25	1.379(3)	.	.	no
C125	H125'	0.94(2)	.	.	no
C25	C26	1.382(3)	.	.	no

C125	H125"	1.02(3)	.	.	no
C125	H125	0.97(3)	.	.	no
C126	H126'	0.90(3)	.	.	no
C126	H126"	0.93(2)	.	.	no
C126	H126	0.93(3)	.	.	no
C27	C28	1.388(3)	.	.	no
C127	H127	0.97(2)	.	.	no
C27	B2	1.663(3)	.	.	yes
C27	C212	1.389(3)	.	.	no
C128	H128	1.02(3)	.	.	no
C128	H128'	0.92(3)	.	.	no
C28	C29	1.382(3)	.	.	no
C128	H128"	1.03(3)	.	.	no
C129	H129'	0.98(3)	.	.	no
C129	H129"	1.10(3)	.	.	no
C129	H129	0.95(3)	.	.	no
C29	C210	1.369(3)	.	.	no
C210	C211	1.378(3)	.	.	no
C211	C212	1.380(3)	.	.	no
C213	C214	1.385(3)	.	.	no
C213	C218	1.387(3)	.	.	no
C213	B2	1.661(3)	.	.	yes
C214	C215	1.374(3)	.	.	no
C215	C216	1.372(3)	.	.	no
C216	C217	1.379(3)	.	.	no
C217	C218	1.381(3)	.	.	no
C219	C220	1.391(3)	.	.	no
C219	C224	1.392(3)	.	.	no
C219	B2	1.648(3)	.	.	yes
C220	C221	1.378(3)	.	.	no
C221	C222	1.366(3)	.	.	no
C222	C223	1.372(3)	.	.	no
C223	C224	1.379(3)	.	.	no

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N11	V1	N12	104.07(8)	.	.	.	yes
N11	V1	C11	144.51(8)	.	.	.	yes
N11	V1	C12	112.30(8)	.	.	.	yes
N11	V1	C13	85.18(8)	.	.	.	yes
N11	V1	C14	93.91(8)	.	.	.	yes
N11	V1	C15	128.52(8)	.	.	.	yes
N11	V1	C114	99.99(8)	.	.	.	yes
N12	V1	C11	96.33(8)	.	.	.	yes
N12	V1	C12	95.56(8)	.	.	.	yes
N12	V1	C13	126.48(8)	.	.	.	yes
N12	V1	C14	153.81(8)	.	.	.	yes
N12	V1	C15	126.60(7)	.	.	.	yes
N12	V1	C114	107.77(7)	.	.	.	yes
C11	V1	C12	35.86(8)	.	.	.	yes
C11	V1	C13	59.40(8)	.	.	.	yes
C11	V1	C14	59.05(8)	.	.	.	yes
C11	V1	C15	35.19(8)	.	.	.	yes
C11	V1	C114	101.00(8)	.	.	.	yes

C12	V1	C13	36.05(9)	.	.	.	yes
C12	V1	C14	59.58(8)	.	.	.	yes
C12	V1	C15	59.46(8)	.	.	.	yes
C12	V1	C114	133.95(8)	.	.	.	yes
C13	V1	C14	35.43(8)	.	.	.	yes
C13	V1	C15	59.24(8)	.	.	.	yes
C13	V1	C114	122.56(8)	.	.	.	yes
C14	V1	C15	35.63(8)	.	.	.	yes
C14	V1	C114	87.24(8)	.	.	.	yes
C15	V1	C114	74.88(7)	.	.	.	yes
V1	N11	C117	157.85(15)	.	.	.	yes
V1	N12	C124	120.54(13)	.	.	.	yes
V1	N12	C127	127.12(13)	.	.	.	yes
C124	N12	C127	111.93(16)	.	.	.	yes
V1	C11	C12	69.89(12)	.	.	.	yes
V1	C11	C15	72.80(12)	.	.	.	yes
C12	C11	C15	107.9(2)	.	.	.	no
V1	C12	C11	74.25(12)	.	.	.	yes
V1	C12	C13	72.46(12)	.	.	.	yes
C11	C12	C13	107.90(19)	.	.	.	no
V1	C13	C12	71.49(13)	.	.	.	yes
V1	C13	C14	73.26(13)	.	.	.	yes
C12	C13	C14	108.3(2)	.	.	.	no
V1	C14	C13	71.31(13)	.	.	.	yes
V1	C14	C15	73.32(12)	.	.	.	yes
C13	C14	C15	108.3(2)	.	.	.	no
V1	C15	C11	72.01(12)	.	.	.	yes
V1	C15	C14	71.05(12)	.	.	.	yes
V1	C15	C16	113.33(14)	.	.	.	yes
C11	C15	C14	107.54(19)	.	.	.	no
C11	C15	C16	124.87(19)	.	.	.	no
C14	C15	C16	126.54(19)	.	.	.	no
C15	C16	C17	111.46(19)	.	.	.	no
C15	C16	C18	110.18(19)	.	.	.	no
C15	C16	C19	102.76(17)	.	.	.	no
C17	C16	C18	108.6(2)	.	.	.	no
C17	C16	C19	110.73(19)	.	.	.	no
C18	C16	C19	113.12(18)	.	.	.	no
C16	C19	C110	123.65(19)	.	.	.	no
C16	C19	C114	118.60(18)	.	.	.	no
C110	C19	C114	117.67(19)	.	.	.	no
C19	C110	C111	121.8(2)	.	.	.	no
C110	C111	C112	119.3(2)	.	.	.	no
C110	C111	C115	119.5(2)	.	.	.	no
C112	C111	C115	121.3(2)	.	.	.	no
C15	C11	H11	124.9(13)	.	.	.	no
V1	C11	H11	119.6(13)	.	.	.	no
C12	C11	H11	127.0(13)	.	.	.	no
C111	C112	C113	121.6(2)	.	.	.	no
V1	C12	H12	117.6(14)	.	.	.	no
C11	C12	H12	124.6(15)	.	.	.	no
C13	C12	H12	127.5(14)	.	.	.	no
V1	C13	H13	118.8(13)	.	.	.	no
C112	C113	C114	118.2(2)	.	.	.	no
C112	C113	C116	121.1(2)	.	.	.	no
C114	C113	C116	120.6(2)	.	.	.	no
C12	C13	H13	123.9(14)	.	.	.	no
C14	C13	H13	127.7(14)	.	.	.	no
V1	C114	C19	93.75(12)	.	.	.	yes
V1	C14	H14	117.0(15)	.	.	.	no
V1	C114	C113	106.71(14)	.	.	.	yes

C19	C114	C113	121.26 (19)	.	.	.	no
C13	C14	H14	125.6 (15)	.	.	.	no
C15	C14	H14	125.9 (15)	.	.	.	no
N11	C117	C118	121.62 (19)	.	.	.	yes
C16	C17	H17	113.3 (16)	.	.	.	no
C16	C17	H17'	110.4 (15)	.	.	.	no
C16	C17	H17"	107.8 (15)	.	.	.	no
N11	C117	C122	119.67 (18)	.	.	.	yes
C118	C117	C122	118.71 (19)	.	.	.	no
H17'	C17	H17"	109 (2)	.	.	.	no
H17	C17	H17"	112 (2)	.	.	.	no
H17	C17	H17'	105 (2)	.	.	.	no
C16	C18	H18"	109.1 (13)	.	.	.	no
C16	C18	H18'	111.1 (14)	.	.	.	no
H18'	C18	H18"	114.8 (19)	.	.	.	no
H18	C18	H18'	108 (2)	.	.	.	no
H18	C18	H18"	106 (2)	.	.	.	no
C117	C118	C119	120.0 (2)	.	.	.	no
C16	C18	H18	108.0 (16)	.	.	.	no
C118	C119	C120	121.8 (2)	.	.	.	no
C119	C120	C121	117.7 (2)	.	.	.	no
C119	C120	C123	120.7 (2)	.	.	.	no
C121	C120	C123	121.6 (2)	.	.	.	no
C120	C121	C122	121.7 (2)	.	.	.	no
C117	C122	C121	120.2 (2)	.	.	.	no
N12	C124	C126	111.65 (19)	.	.	.	yes
C125	C124	C126	110.74 (19)	.	.	.	no
N12	C124	C125	112.02 (18)	.	.	.	yes
C128	C127	C129	112.3 (2)	.	.	.	no
N12	C127	C128	110.75 (18)	.	.	.	yes
N12	C127	C129	111.85 (18)	.	.	.	yes
C19	C110	H110	121.1 (14)	.	.	.	no
C111	C110	H110	117.1 (14)	.	.	.	no
C111	C112	H112	120.5 (16)	.	.	.	no
C113	C112	H112	117.8 (16)	.	.	.	no
V1	C114	H114	81.4 (14)	.	.	.	no
C19	C114	H114	119.5 (15)	.	.	.	no
C113	C114	H114	117.7 (14)	.	.	.	no
C111	C115	H115'	110 (2)	.	.	.	no
C111	C115	H115"	111 (2)	.	.	.	no
C111	C115	H115	112 (2)	.	.	.	no
H115'	C115	H115"	114 (3)	.	.	.	no
H115'	C115	H115	106 (3)	.	.	.	no
H115"	C115	H115	104 (3)	.	.	.	no
C113	C116	H116'	116.0 (18)	.	.	.	no
C113	C116	H116"	108 (2)	.	.	.	no
C113	C116	H116	109.5 (18)	.	.	.	no
H116'	C116	H116"	112 (3)	.	.	.	no
H116'	C116	H116	109 (3)	.	.	.	no
H116"	C116	H116	102 (3)	.	.	.	no
C117	C118	H118	114.8 (15)	.	.	.	no
C119	C118	H118	125.2 (16)	.	.	.	no
C118	C119	H119	117.6 (17)	.	.	.	no
C120	C119	H119	120.5 (17)	.	.	.	no
C120	C121	H121	119.2 (17)	.	.	.	no
C122	C121	H121	119.2 (17)	.	.	.	no
C22	C21	C26	113.12 (18)	.	.	.	no
C22	C21	B2	127.13 (17)	.	.	.	yes
C26	C21	B2	119.10 (17)	.	.	.	yes
F22	C22	C21	120.83 (18)	.	.	.	yes
F22	C22	C23	114.88 (17)	.	.	.	yes

C21	C22	C23	124.28(18)	.	.	.	no
C117	C122	H122	117.5(14)	.	.	.	no
C121	C122	H122	122.3(14)	.	.	.	no
H123'	C123	H123	98(3)	.	.	.	no
C120	C123	H123'	109(3)	.	.	.	no
C120	C123	H123"	108(3)	.	.	.	no
C120	C123	H123	109(2)	.	.	.	no
H123'	C123	H123"	134(4)	.	.	.	no
F23	C23	C22	120.54(18)	.	.	.	yes
F23	C23	C24	119.87(18)	.	.	.	yes
C22	C23	C24	119.59(19)	.	.	.	no
H123"	C123	H123	94(4)	.	.	.	no
F24	C24	C25	120.18(18)	.	.	.	yes
C23	C24	C25	119.22(19)	.	.	.	no
C126	C124	H124	107.5(11)	.	.	.	no
F24	C24	C23	120.60(18)	.	.	.	yes
N12	C124	H124	107.6(12)	.	.	.	no
C125	C124	H124	107.0(11)	.	.	.	no
F25	C25	C26	120.96(18)	.	.	.	yes
C24	C25	C26	118.87(18)	.	.	.	no
C124	C125	H125	109.1(17)	.	.	.	no
F25	C25	C24	120.18(18)	.	.	.	yes
C124	C125	H125'	106.6(14)	.	.	.	no
C124	C125	H125"	110.0(14)	.	.	.	no
H125"	C125	H125	110(2)	.	.	.	no
H125'	C125	H125"	114(2)	.	.	.	no
H125'	C125	H125	108(2)	.	.	.	no
H126"	C126	H126	111(2)	.	.	.	no
C124	C126	H126'	105.7(17)	.	.	.	no
C124	C126	H126"	112.9(14)	.	.	.	no
C124	C126	H126	111.0(15)	.	.	.	no
H126'	C126	H126"	110(2)	.	.	.	no
H126'	C126	H126	107(2)	.	.	.	no
F26	C26	C25	115.47(17)	.	.	.	yes
C21	C26	C25	124.88(18)	.	.	.	no
F26	C26	C21	119.62(17)	.	.	.	yes
C28	C27	B2	127.30(18)	.	.	.	yes
C212	C27	B2	119.79(17)	.	.	.	yes
C129	C127	H127	108.7(12)	.	.	.	no
N12	C127	H127	105.5(12)	.	.	.	no
C128	C127	H127	107.3(12)	.	.	.	no
C28	C27	C212	112.55(18)	.	.	.	no
H128'	C128	H128"	115(2)	.	.	.	no
H128'	C128	H128	109(2)	.	.	.	no
C127	C128	H128	110.2(16)	.	.	.	no
C127	C128	H128'	107.3(16)	.	.	.	no
C127	C128	H128"	106.5(14)	.	.	.	no
F28	C28	C27	120.74(17)	.	.	.	yes
H128"	C128	H128	110(2)	.	.	.	no
C27	C28	C29	124.7(2)	.	.	.	no
F28	C28	C29	114.59(18)	.	.	.	yes
C127	C129	H129"	106.8(15)	.	.	.	no
C127	C129	H129	114.0(15)	.	.	.	no
H129'	C129	H129	110(2)	.	.	.	no
H129"	C129	H129	106(2)	.	.	.	no
H129'	C129	H129"	114(2)	.	.	.	no
C127	C129	H129'	106.6(16)	.	.	.	no
F29	C29	C28	120.39(19)	.	.	.	yes
F29	C29	C210	120.01(19)	.	.	.	yes
C28	C29	C210	119.6(2)	.	.	.	no
F210	C210	C29	120.6(2)	.	.	.	yes

F210	C210	C211	120.4(2)	.	.	.	yes
C29	C210	C211	119.1(2)	.	.	.	no
F211	C211	C210	120.07(19)	.	.	.	yes
F211	C211	C212	120.97(19)	.	.	.	yes
C210	C211	C212	119.0(2)	.	.	.	no
F212	C212	C27	119.11(17)	.	.	.	yes
F212	C212	C211	115.72(18)	.	.	.	yes
C27	C212	C211	125.2(2)	.	.	.	no
C214	C213	C218	112.83(18)	.	.	.	no
C214	C213	B2	120.19(17)	.	.	.	yes
C218	C213	B2	126.75(18)	.	.	.	yes
F214	C214	C213	119.23(17)	.	.	.	yes
F214	C214	C215	115.73(18)	.	.	.	yes
C213	C214	C215	125.04(19)	.	.	.	no
F215	C215	C214	121.08(19)	.	.	.	yes
F215	C215	C216	119.34(19)	.	.	.	yes
C214	C215	C216	119.6(2)	.	.	.	no
F216	C216	C215	120.9(2)	.	.	.	yes
F216	C216	C217	120.6(2)	.	.	.	yes
C215	C216	C217	118.49(19)	.	.	.	no
F217	C217	C216	119.69(18)	.	.	.	yes
F217	C217	C218	120.7(2)	.	.	.	yes
C216	C217	C218	119.6(2)	.	.	.	no
F218	C218	C213	120.90(17)	.	.	.	yes
F218	C218	C217	114.68(18)	.	.	.	yes
C213	C218	C217	124.4(2)	.	.	.	no
C220	C219	C224	113.05(18)	.	.	.	no
C220	C219	B2	119.50(17)	.	.	.	yes
C224	C219	B2	127.18(17)	.	.	.	yes
F220	C220	C219	119.31(17)	.	.	.	yes
F220	C220	C221	116.24(17)	.	.	.	yes
C219	C220	C221	124.43(19)	.	.	.	no
F221	C221	C220	120.41(18)	.	.	.	yes
F221	C221	C222	120.26(19)	.	.	.	yes
C220	C221	C222	119.33(19)	.	.	.	no
F222	C222	C221	120.5(2)	.	.	.	yes
F222	C222	C223	120.1(2)	.	.	.	yes
C221	C222	C223	119.4(2)	.	.	.	no
F223	C223	C222	120.14(18)	.	.	.	yes
F223	C223	C224	120.43(18)	.	.	.	yes
C222	C223	C224	119.43(19)	.	.	.	no
F224	C224	C219	120.89(17)	.	.	.	yes
F224	C224	C223	114.95(17)	.	.	.	yes
C219	C224	C223	124.15(19)	.	.	.	no
C21	B2	C27	114.78(16)	.	.	.	yes
C21	B2	C213	113.44(16)	.	.	.	yes
C21	B2	C219	101.42(15)	.	.	.	yes
C27	B2	C213	101.38(15)	.	.	.	yes
C27	B2	C219	112.60(16)	.	.	.	yes
C213	B2	C219	113.79(16)	.	.	.	yes

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N12	V1	N11	C117	146.0(4)	.	.	.	.	no
C11	V1	N11	C117	22.8(5)	.	.	.	.	no
C12	V1	N11	C117	43.8(4)	.	.	.	.	no
C13	V1	N11	C117	19.5(4)	.	.	.	.	no
C14	V1	N11	C117	-14.8(4)	.	.	.	.	no
C15	V1	N11	C117	-24.1(4)	.	.	.	.	no
C114	V1	N11	C117	-102.7(4)	.	.	.	.	no
N11	V1	N12	C124	177.20(14)	.	.	.	.	no
N11	V1	N12	C127	-10.80(17)	.	.	.	.	no
C11	V1	N12	C124	-32.07(15)	.	.	.	.	no
C11	V1	N12	C127	139.94(16)	.	.	.	.	no
C12	V1	N12	C124	-68.13(15)	.	.	.	.	no
C12	V1	N12	C127	103.88(16)	.	.	.	.	no
C13	V1	N12	C124	-88.36(16)	.	.	.	.	no
C13	V1	N12	C127	83.65(18)	.	.	.	.	no
C14	V1	N12	C124	-50.8(2)	.	.	.	.	no
C14	V1	N12	C127	121.2(2)	.	.	.	.	no
C15	V1	N12	C124	-12.43(18)	.	.	.	.	no
C15	V1	N12	C127	159.58(14)	.	.	.	.	no
C114	V1	N12	C124	71.64(15)	.	.	.	.	no
C114	V1	N12	C127	-116.35(16)	.	.	.	.	no
N11	V1	C11	C12	34.5(2)	.	.	.	.	no
N11	V1	C11	C15	-82.68(17)	.	.	.	.	no
N12	V1	C11	C12	-90.74(14)	.	.	.	.	no
N12	V1	C11	C15	152.09(12)	.	.	.	.	no
C12	V1	C11	C15	-117.18(19)	.	.	.	.	no
C13	V1	C11	C12	38.26(14)	.	.	.	.	no
C13	V1	C11	C15	-78.92(14)	.	.	.	.	no
C14	V1	C11	C12	79.74(15)	.	.	.	.	no
C14	V1	C11	C15	-37.44(12)	.	.	.	.	no
C15	V1	C11	C12	117.18(19)	.	.	.	.	no
C114	V1	C11	C12	159.73(14)	.	.	.	.	no
C114	V1	C11	C15	42.55(13)	.	.	.	.	no
N11	V1	C12	C11	-159.19(13)	.	.	.	.	no
N11	V1	C12	C13	-44.10(15)	.	.	.	.	no
N12	V1	C12	C11	93.12(14)	.	.	.	.	no
N12	V1	C12	C13	-151.80(13)	.	.	.	.	no
C11	V1	C12	C13	115.08(19)	.	.	.	.	no
C13	V1	C12	C11	-115.08(19)	.	.	.	.	no
C14	V1	C12	C11	-78.12(14)	.	.	.	.	no
C14	V1	C12	C13	36.96(13)	.	.	.	.	no
C15	V1	C12	C11	-36.53(13)	.	.	.	.	no
C15	V1	C12	C13	78.55(14)	.	.	.	.	no
C114	V1	C12	C11	-28.19(18)	.	.	.	.	no
C114	V1	C12	C13	86.89(15)	.	.	.	.	no
N11	V1	C13	C12	139.75(14)	.	.	.	.	no
N11	V1	C13	C14	-103.70(14)	.	.	.	.	no
N12	V1	C13	C12	35.80(16)	.	.	.	.	no
N12	V1	C13	C14	152.36(13)	.	.	.	.	no
C11	V1	C13	C12	-38.06(13)	.	.	.	.	no
C11	V1	C13	C14	78.50(14)	.	.	.	.	no
C12	V1	C13	C14	116.56(19)	.	.	.	.	no
C14	V1	C13	C12	-116.56(19)	.	.	.	.	no
C15	V1	C13	C12	-79.22(14)	.	.	.	.	no
C15	V1	C13	C14	37.34(13)	.	.	.	.	no
C114	V1	C13	C12	-121.47(13)	.	.	.	.	no
C114	V1	C13	C14	-4.91(17)	.	.	.	.	no
N11	V1	C14	C13	76.02(14)	.	.	.	.	no
N11	V1	C14	C15	-167.45(13)	.	.	.	.	no
N12	V1	C14	C13	-57.7(2)	.	.	.	.	no

N12	V1	C14	C15	58.8(2)	.	.	.	.	no
C11	V1	C14	C13	-79.57(14)	.	.	.	.	no
C11	V1	C14	C15	36.96(12)	.	.	.	.	no
C12	V1	C14	C13	-37.62(13)	.	.	.	.	no
C12	V1	C14	C15	78.92(14)	.	.	.	.	no
C13	V1	C14	C15	116.53(19)	.	.	.	.	no
C15	V1	C14	C13	-116.53(19)	.	.	.	.	no
C114	V1	C14	C13	175.86(14)	.	.	.	.	no
C114	V1	C14	C15	-67.61(13)	.	.	.	.	no
N11	V1	C15	C11	132.61(13)	.	.	.	.	no
N11	V1	C15	C14	16.09(16)	.	.	.	.	no
N11	V1	C15	C16	-106.43(16)	.	.	.	.	no
N12	V1	C15	C11	-35.42(15)	.	.	.	.	no
N12	V1	C15	C14	-151.94(12)	.	.	.	.	no
N12	V1	C15	C16	85.55(16)	.	.	.	.	no
C11	V1	C15	C14	-116.52(18)	.	.	.	.	no
C11	V1	C15	C16	121.0(2)	.	.	.	.	no
C12	V1	C15	C11	37.24(13)	.	.	.	.	no
C12	V1	C15	C14	-79.28(14)	.	.	.	.	no
C12	V1	C15	C16	158.21(18)	.	.	.	.	no
C13	V1	C15	C11	79.39(14)	.	.	.	.	no
C13	V1	C15	C14	-37.12(13)	.	.	.	.	no
C13	V1	C15	C16	-159.64(18)	.	.	.	.	no
C14	V1	C15	C11	116.52(18)	.	.	.	.	no
C14	V1	C15	C16	-122.5(2)	.	.	.	.	no
C114	V1	C15	C11	-136.55(14)	.	.	.	.	no
C114	V1	C15	C14	106.93(13)	.	.	.	.	no
C114	V1	C15	C16	-15.59(14)	.	.	.	.	no
N11	V1	C114	C19	165.89(13)	.	.	.	.	no
N11	V1	C114	C113	-69.88(15)	.	.	.	.	no
N12	V1	C114	C19	-85.72(14)	.	.	.	.	no
N12	V1	C114	C113	38.52(16)	.	.	.	.	no
C11	V1	C114	C19	14.67(14)	.	.	.	.	no
C11	V1	C114	C113	138.91(15)	.	.	.	.	no
C12	V1	C114	C19	31.05(18)	.	.	.	.	no
C12	V1	C114	C113	155.28(14)	.	.	.	.	no
C13	V1	C114	C19	75.24(15)	.	.	.	.	no
C13	V1	C114	C113	-160.52(14)	.	.	.	.	no
C14	V1	C114	C19	72.40(14)	.	.	.	.	no
C14	V1	C114	C113	-163.37(15)	.	.	.	.	no
C15	V1	C114	C19	38.48(13)	.	.	.	.	no
C15	V1	C114	C113	162.72(16)	.	.	.	.	no
V1	N11	C117	C118	-104.5(4)	.	.	.	.	no
V1	N11	C117	C122	75.2(4)	.	.	.	.	no
V1	N12	C124	C125	106.39(19)	.	.	.	.	no
V1	N12	C124	C126	-128.76(18)	.	.	.	.	no
C127	N12	C124	C125	-66.8(2)	.	.	.	.	no
C127	N12	C124	C126	58.1(2)	.	.	.	.	no
V1	N12	C127	C128	-63.9(2)	.	.	.	.	no
V1	N12	C127	C129	62.3(2)	.	.	.	.	no
C124	N12	C127	C128	108.7(2)	.	.	.	.	no
C124	N12	C127	C129	-125.17(19)	.	.	.	.	no
V1	C11	C12	C13	-65.16(15)	.	.	.	.	no
C15	C11	C12	V1	63.29(15)	.	.	.	.	no
C15	C11	C12	C13	-1.9(2)	.	.	.	.	no
V1	C11	C15	C14	62.57(15)	.	.	.	.	no
V1	C11	C15	C16	-106.3(2)	.	.	.	.	no
C12	C11	C15	V1	-61.41(15)	.	.	.	.	no
C12	C11	C15	C14	1.2(2)	.	.	.	.	no
C12	C11	C15	C16	-167.7(2)	.	.	.	.	no
V1	C12	C13	C14	-64.47(16)	.	.	.	.	no

C11	C12	C13	V1	66.35(15)	.	.	.	.	no
C11	C12	C13	C14	1.9(3)	.	.	.	.	no
V1	C13	C14	C15	-64.48(15)	.	.	.	.	no
C12	C13	C14	V1	63.33(16)	.	.	.	.	no
C12	C13	C14	C15	-1.2(3)	.	.	.	.	no
V1	C14	C15	C11	-63.19(15)	.	.	.	.	no
V1	C14	C15	C16	105.5(2)	.	.	.	.	no
C13	C14	C15	V1	63.18(16)	.	.	.	.	no
C13	C14	C15	C11	0.0(2)	.	.	.	.	no
C13	C14	C15	C16	168.7(2)	.	.	.	.	no
V1	C15	C16	C17	107.99(18)	.	.	.	.	no
V1	C15	C16	C18	-131.44(16)	.	.	.	.	no
V1	C15	C16	C19	-10.63(19)	.	.	.	.	no
C11	C15	C16	C17	-168.3(2)	.	.	.	.	no
C11	C15	C16	C18	-47.7(3)	.	.	.	.	no
C11	C15	C16	C19	73.1(2)	.	.	.	.	no
C14	C15	C16	C17	24.9(3)	.	.	.	.	no
C14	C15	C16	C18	145.5(2)	.	.	.	.	no
C14	C15	C16	C19	-93.7(2)	.	.	.	.	no
C15	C16	C19	C110	-117.6(2)	.	.	.	.	no
C15	C16	C19	C114	59.1(2)	.	.	.	.	no
C17	C16	C19	C110	123.3(2)	.	.	.	.	no
C17	C16	C19	C114	-60.0(3)	.	.	.	.	no
C18	C16	C19	C110	1.2(3)	.	.	.	.	no
C18	C16	C19	C114	177.86(19)	.	.	.	.	no
C16	C19	C110	C111	178.9(2)	.	.	.	.	no
C114	C19	C110	C111	2.2(3)	.	.	.	.	no
C16	C19	C114	V1	-68.62(18)	.	.	.	.	no
C110	C19	C114	V1	108.27(17)	.	.	.	.	no
C16	C19	C114	C113	179.25(19)	.	.	.	.	no
C110	C19	C114	C113	-3.9(3)	.	.	.	.	no
C26	C21	C22	F22	-177.61(17)	.	.	.	.	no
C26	C21	C22	C23	1.8(3)	.	.	.	.	no
B2	C21	C22	F22	-7.1(3)	.	.	.	.	no
B2	C21	C22	C23	172.30(19)	.	.	.	.	no
C22	C21	C26	F26	178.04(17)	.	.	.	.	no
C22	C21	C26	C25	-0.2(3)	.	.	.	.	no
B2	C21	C26	F26	6.7(3)	.	.	.	.	no
B2	C21	C26	C25	-171.53(19)	.	.	.	.	no
C22	C21	B2	C27	19.3(3)	.	.	.	.	no
C22	C21	B2	C213	135.3(2)	.	.	.	.	no
C22	C21	B2	C219	-102.3(2)	.	.	.	.	no
C26	C21	B2	C27	-170.64(17)	.	.	.	.	no
C26	C21	B2	C213	-54.7(2)	.	.	.	.	no
C26	C21	B2	C219	67.7(2)	.	.	.	.	no
F22	C22	C23	F23	-2.3(3)	.	.	.	.	no
F22	C22	C23	C24	176.87(18)	.	.	.	.	no
C21	C22	C23	F23	178.29(18)	.	.	.	.	no
C21	C22	C23	C24	-2.6(3)	.	.	.	.	no
F23	C23	C24	F24	0.7(3)	.	.	.	.	no
F23	C23	C24	C25	-179.26(18)	.	.	.	.	no
C22	C23	C24	F24	-178.51(18)	.	.	.	.	no
C22	C23	C24	C25	1.6(3)	.	.	.	.	no
F24	C24	C25	F25	0.5(3)	.	.	.	.	no
F24	C24	C25	C26	-180.00(18)	.	.	.	.	no
C23	C24	C25	F25	-179.60(18)	.	.	.	.	no
C23	C24	C25	C26	-0.1(3)	.	.	.	.	no
F25	C25	C26	F26	0.6(3)	.	.	.	.	no
F25	C25	C26	C21	178.87(18)	.	.	.	.	no
C24	C25	C26	F26	-178.92(18)	.	.	.	.	no
C24	C25	C26	C21	-0.7(3)	.	.	.	.	no

C212	C27	C28	F28	178.35(17)	.	.	.	.	no
C212	C27	C28	C29	-0.5(3)	.	.	.	.	no
B2	C27	C28	F28	5.3(3)	.	.	.	.	no
B2	C27	C28	C29	-173.5(2)	.	.	.	.	no
C28	C27	B2	C21	-134.0(2)	.	.	.	.	no
C28	C27	B2	C213	103.4(2)	.	.	.	.	no
C28	C27	B2	C219	-18.6(3)	.	.	.	.	no
C212	C27	B2	C21	53.4(2)	.	.	.	.	no
C212	C27	B2	C213	-69.3(2)	.	.	.	.	no
C212	C27	B2	C219	168.79(18)	.	.	.	.	no
C28	C27	C212	C211	0.6(3)	.	.	.	.	no
C28	C27	C212	F212	-178.93(17)	.	.	.	.	no
B2	C27	C212	F212	-5.3(3)	.	.	.	.	no
B2	C27	C212	C211	174.27(19)	.	.	.	.	no
F28	C28	C29	F29	0.9(3)	.	.	.	.	no
C27	C28	C29	C210	0.2(3)	.	.	.	.	no
F28	C28	C29	C210	-178.73(18)	.	.	.	.	no
C27	C28	C29	F29	179.82(19)	.	.	.	.	no
C28	C29	C210	F210	179.20(19)	.	.	.	.	no
F29	C29	C210	C211	-179.59(19)	.	.	.	.	no
C28	C29	C210	C211	0.1(3)	.	.	.	.	no
F29	C29	C210	F210	-0.5(3)	.	.	.	.	no
F210	C210	C211	F211	1.2(3)	.	.	.	.	no
F210	C210	C211	C212	-179.06(19)	.	.	.	.	no
C29	C210	C211	F211	-179.69(19)	.	.	.	.	no
C29	C210	C211	C212	0.1(3)	.	.	.	.	no
F211	C211	C212	C27	179.30(19)	.	.	.	.	no
C210	C211	C212	F212	179.12(18)	.	.	.	.	no
C210	C211	C212	C27	-0.5(3)	.	.	.	.	no
F211	C211	C212	F212	-1.1(3)	.	.	.	.	no
C218	C213	C214	F214	-178.95(17)	.	.	.	.	no
C218	C213	C214	C215	1.0(3)	.	.	.	.	no
B2	C213	C214	F214	-4.1(3)	.	.	.	.	no
B2	C213	C214	C215	175.86(19)	.	.	.	.	no
C214	C213	C218	F218	-179.42(17)	.	.	.	.	no
C214	C213	C218	C217	-0.4(3)	.	.	.	.	no
B2	C213	C218	F218	6.1(3)	.	.	.	.	no
B2	C213	C218	C217	-174.93(19)	.	.	.	.	no
C214	C213	B2	C21	164.65(17)	.	.	.	.	no
C214	C213	B2	C27	-71.8(2)	.	.	.	.	no
C214	C213	B2	C219	49.4(2)	.	.	.	.	no
C218	C213	B2	C21	-21.2(3)	.	.	.	.	no
C218	C213	B2	C27	102.4(2)	.	.	.	.	no
C218	C213	B2	C219	-136.5(2)	.	.	.	.	no
F214	C214	C215	F215	-1.4(3)	.	.	.	.	no
F214	C214	C215	C216	178.92(18)	.	.	.	.	no
C213	C214	C215	F215	178.70(19)	.	.	.	.	no
C213	C214	C215	C216	-1.0(3)	.	.	.	.	no
F215	C215	C216	F216	-0.4(3)	.	.	.	.	no
F215	C215	C216	C217	-179.29(18)	.	.	.	.	no
C214	C215	C216	F216	179.31(19)	.	.	.	.	no
C214	C215	C216	C217	0.4(3)	.	.	.	.	no
F216	C216	C217	F217	0.4(3)	.	.	.	.	no
F216	C216	C217	C218	-178.83(18)	.	.	.	.	no
C215	C216	C217	F217	179.27(18)	.	.	.	.	no
C215	C216	C217	C218	0.1(3)	.	.	.	.	no
F217	C217	C218	F218	-0.2(3)	.	.	.	.	no
F217	C217	C218	C213	-179.24(18)	.	.	.	.	no
C216	C217	C218	F218	179.00(18)	.	.	.	.	no
C216	C217	C218	C213	0.0(3)	.	.	.	.	no
C224	C219	C220	F220	176.59(17)	.	.	.	.	no

C224	C219	C220	C221	-5.0(3)	.	.	.	.	no
B2	C219	C220	F220	2.1(3)	.	.	.	.	no
B2	C219	C220	C221	-179.44(19)	.	.	.	.	no
C220	C219	C224	F224	-176.86(17)	.	.	.	.	no
C220	C219	C224	C223	4.2(3)	.	.	.	.	no
B2	C219	C224	F224	-2.9(3)	.	.	.	.	no
B2	C219	C224	C223	178.1(2)	.	.	.	.	no
C220	C219	B2	C21	70.6(2)	.	.	.	.	no
C220	C219	B2	C27	-52.6(2)	.	.	.	.	no
C220	C219	B2	C213	-167.25(17)	.	.	.	.	no
C224	C219	B2	C21	-103.1(2)	.	.	.	.	no
C224	C219	B2	C27	133.8(2)	.	.	.	.	no
C224	C219	B2	C213	19.1(3)	.	.	.	.	no
F220	C220	C221	F221	0.3(3)	.	.	.	.	no
F220	C220	C221	C222	-178.90(18)	.	.	.	.	no
C219	C220	C221	F221	-178.20(19)	.	.	.	.	no
C219	C220	C221	C222	2.6(3)	.	.	.	.	no
F221	C221	C222	F222	0.9(3)	.	.	.	.	no
F221	C221	C222	C223	-178.20(19)	.	.	.	.	no
C220	C221	C222	F222	-179.91(19)	.	.	.	.	no
C220	C221	C222	C223	1.0(3)	.	.	.	.	no
F222	C222	C223	F223	-0.5(3)	.	.	.	.	no
F222	C222	C223	C224	179.17(18)	.	.	.	.	no
C221	C222	C223	F223	178.65(19)	.	.	.	.	no
C221	C222	C223	C224	-1.7(3)	.	.	.	.	no
F223	C223	C224	F224	-0.5(3)	.	.	.	.	no
F223	C223	C224	C219	178.58(18)	.	.	.	.	no
C222	C223	C224	F224	179.92(18)	.	.	.	.	no
C222	C223	C224	C219	-1.1(3)	.	.	.	.	no

loop_

_geom_contact_atom_site_label_1

_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

_geom_contact_publ_flag

V1	H116'	3.51(3)	.	.	.	no
V1	H128"	3.09(2)	.	.	.	no
V1	H129	3.25(2)	.	.	.	no
F22	F212	2.8126(17)	.	.	.	no
F22	C115	3.182(3)	.	2_555	.	no
F22	F23	2.6449(18)	.	.	.	no
F22	C212	2.830(2)	.	.	.	no
F22	F220	2.8632(18)	.	.	.	no
F22	C27	2.862(2)	.	.	.	no
F23	F24	2.7271(18)	.	.	.	no
F23	F22	2.6449(18)	.	.	.	no
F24	F23	2.7271(18)	.	.	.	no
F24	C18	3.364(3)	.	1_655	.	no
F24	F25	2.7278(18)	.	.	.	no
F25	F26	2.6539(18)	.	.	.	no
F25	F24	2.7278(18)	.	.	.	no
F26	F218	2.8943(17)	.	.	.	no
F26	C213	2.951(2)	.	.	.	no
F26	C219	3.096(2)	.	.	.	no
F26	C218	3.063(2)	.	.	.	no
F26	C224	3.099(2)	.	.	.	no
F26	F224	2.8134(17)	.	.	.	no
F26	F25	2.6539(18)	.	.	.	no
F26	C12	3.352(3)	.	2_545	.	no

F26	F222	3.1151(18)	.	3_656	no
F28	F220	2.8162(18)	.	.	no
F28	C14	3.236(3)	.	.	no
F28	F29	2.6258(18)	.	.	no
F28	C219	2.815(2)	.	.	no
F28	F214	2.9402(16)	.	.	no
F28	C220	2.749(2)	.	.	no
F29	F210	2.727(2)	.	.	no
F29	F28	2.6258(18)	.	.	no
F22	H115	2.47(3)	.	2_555	no
F22	H125'	2.71(2)	.	1_655	no
F22	H112	2.81(2)	.	2_555	no
F23	H123	2.84(4)	.	4_555	no
F24	H18'	2.86(2)	.	3_656	no
F24	H110	2.65(2)	.	1_655	no
F24	H18"	2.71(3)	.	1_655	no
F25	H128	2.83(3)	.	2_545	no
F26	H128	2.81(3)	.	2_545	no
F26	H12	2.46(2)	.	2_545	no
F28	H14	2.44(3)	.	.	no
F29	H13	2.82(2)	.	.	no
F210	F211	2.733(2)	.	.	no
F210	C110	3.235(3)	.	2_555	no
F210	F29	2.727(2)	.	.	no
F211	F210	2.733(2)	.	.	no
F211	F212	2.6626(17)	.	.	no
F212	F218	2.8707(16)	.	.	no
F212	C22	3.057(2)	.	.	no
F212	F211	2.6626(17)	.	.	no
F212	F22	2.8126(17)	.	.	no
F212	C21	2.980(2)	.	.	no
F212	C218	3.126(2)	.	.	no
F212	C126	3.303(3)	.	1_655	no
F212	C213	3.131(2)	.	.	no
F214	C27	3.178(2)	.	.	no
F214	F224	2.7348(17)	.	.	no
F214	F215	2.6638(18)	.	.	no
F214	C219	2.912(2)	.	.	no
F214	C122	3.224(3)	.	.	no
F214	C224	2.926(2)	.	.	no
F214	C28	3.208(2)	.	.	no
F214	F28	2.9402(16)	.	.	no
F215	C116	3.326(3)	.	.	no
F215	F216	2.724(2)	.	.	no
F215	F214	2.6638(18)	.	.	no
F216	F215	2.724(2)	.	.	no
F216	F217	2.727(2)	.	.	no
F217	C123	3.261(3)	.	3_655	no
F217	F216	2.727(2)	.	.	no
F217	C11	3.355(3)	.	2_545	no
F217	F218	2.6334(17)	.	.	no
F218	C26	2.855(2)	.	.	no
F218	C126	3.325(3)	.	1_655	no
F218	F217	2.6334(17)	.	.	no
F218	F26	2.8943(17)	.	.	no
F218	F212	2.8707(16)	.	.	no
F218	C21	2.835(2)	.	.	no
F220	F28	2.8162(18)	.	.	no
F220	C28	3.011(2)	.	.	no
F220	C21	3.108(2)	.	.	no
F220	F221	2.6591(19)	.	.	no

F220	F22	2.8632(18)	.	.	no
F220	C27	2.933(2)	.	.	no
F220	C22	3.102(2)	.	.	no
F221	C223	3.367(3)	.	3_656	no
F221	F222	2.7271(19)	.	.	no
F221	F223	3.1162(19)	.	3_656	no
F221	C128	3.020(3)	.	4_555	no
F221	F220	2.6591(19)	.	.	no
F222	F223	2.7234(19)	.	.	no
F222	F26	3.1151(18)	.	3_656	no
F222	F221	2.7271(19)	.	.	no
F222	C26	2.953(2)	.	3_656	no
F222	C25	2.987(2)	.	3_656	no
F223	F222	2.7234(19)	.	.	no
F223	F224	2.6318(18)	.	.	no
F223	F221	3.1162(19)	.	3_656	no
F224	C214	2.764(2)	.	.	no
F224	C12	3.172(2)	.	2_545	no
F224	F26	2.8134(17)	.	.	no
F224	C13	2.980(2)	.	2_545	no
F224	F214	2.7348(17)	.	.	no
F224	C213	2.846(2)	.	.	no
F224	F223	2.6318(18)	.	.	no
F210	H17'	2.75(3)	.	2_555	no
F210	H123	2.81(4)	.	.	no
F211	H115"	2.70(4)	.	2_555	no
F212	H126	2.87(3)	.	1_655	no
F214	H17	2.87(3)	.	.	no
F214	H122	2.38(2)	.	.	no
F215	H122	2.75(2)	.	.	no
F215	H116'	2.87(3)	.	.	no
F218	H126'	2.68(3)	.	1_655	no
F221	H118	2.59(3)	.	4_555	no
F221	H128"	2.64(3)	.	4_555	no
F221	H128'	2.80(3)	.	4_555	no
F223	H17'	2.76(3)	.	.	no
F224	H12	2.85(2)	.	2_545	no
F224	H13	2.38(2)	.	2_545	no
N11	C128	3.417(3)	.	.	no
N11	N12	2.799(2)	.	.	no
N11	C12	3.294(3)	.	.	no
N11	C13	2.716(3)	.	.	no
N11	C14	2.943(3)	.	.	no
N11	C114	3.167(3)	.	.	no
N11	C129	3.166(3)	.	.	no
N11	C127	3.215(3)	.	.	no
N12	C11	3.141(3)	.	.	no
N12	C12	3.077(3)	.	.	no
N12	N11	2.799(2)	.	.	no
N11	H116'	2.86(3)	.	.	no
N11	H129	2.50(3)	.	.	no
N11	H114	2.84(2)	.	.	no
N11	H128"	2.67(3)	.	.	no
N11	H13	2.77(2)	.	.	no
C11	C124	3.207(3)	.	.	no
C11	N12	3.141(3)	.	.	no
C11	C13	2.283(3)	.	.	no
C11	C14	2.283(3)	.	.	no
C11	F217	3.355(3)	.	2_555	no
C11	C216	3.383(3)	.	2_555	no
C11	C125	3.546(4)	.	.	no

C11	C217	3.308(3)	.	2_555	no
C11	C16	2.596(3)	.	.	no
C11	C19	3.107(3)	.	.	no
C12	C14	2.274(3)	.	.	no
C12	C217	3.283(3)	.	2_555	no
C12	C218	3.472(3)	.	2_555	no
C12	F26	3.352(3)	.	2_555	no
C12	C216	3.376(3)	.	2_555	no
C12	N11	3.294(3)	.	.	no
C12	N12	3.077(3)	.	.	no
C12	C15	2.285(3)	.	.	no
C12	C124	3.564(3)	.	.	no
C12	F224	3.172(2)	.	2_555	no
C13	N11	2.716(3)	.	.	no
C13	C15	2.283(3)	.	.	no
C13	C11	2.283(3)	.	.	no
C13	C117	3.300(3)	.	.	no
C13	F224	2.980(2)	.	2_555	no
C14	C16	2.625(3)	.	.	no
C14	N11	2.943(3)	.	.	no
C14	C19	3.326(3)	.	.	no
C14	C114	3.256(3)	.	.	no
C14	C11	2.283(3)	.	.	no
C14	C12	2.274(3)	.	.	no
C14	F28	3.236(3)	.	.	no
C15	C12	2.285(3)	.	.	no
C15	C19	2.384(3)	.	.	no
C15	C13	2.283(3)	.	.	no
C15	C114	2.887(3)	.	.	no
C17	C222	3.476(3)	.	.	no
C17	C223	3.275(3)	.	.	no
C18	F24	3.364(3)	.	1_455	no
C21	F218	2.835(2)	.	.	no
C21	F220	3.108(2)	.	.	no
C21	F212	2.980(2)	.	.	no
C22	C212	3.419(3)	.	.	no
C22	F212	3.057(2)	.	.	no
C22	F220	3.102(2)	.	.	no
C25	F222	2.987(2)	.	3_656	no
C26	C218	3.398(3)	.	.	no
C26	F218	2.855(2)	.	.	no
C26	F222	2.953(2)	.	3_656	no
C27	F220	2.933(2)	.	.	no
C27	F22	2.862(2)	.	.	no
C27	F214	3.178(2)	.	.	no
C28	F220	3.011(2)	.	.	no
C28	C220	3.326(3)	.	.	no
C28	F214	3.208(2)	.	.	no
C29	C121	3.496(3)	.	.	no
C110	C210	3.499(3)	.	2_545	no
C110	F210	3.235(3)	.	2_545	no
C11	H125	2.97(3)	.	.	no
C11	H124	2.64(2)	.	.	no
C111	C126	3.419(4)	.	.	no
C11	H18"	2.68(2)	.	.	no
C111	C210	3.510(3)	.	2_545	no
C11	H12	2.08(2)	.	.	no
C12	H11	2.11(2)	.	.	no
C12	H13	2.10(2)	.	.	no
C12	H125	2.89(3)	.	.	no
C13	H14	2.09(3)	.	.	no

C13	H12	2.10(2)	.	.	no
C14	H114	2.81(2)	.	.	no
C114	C16	2.538(3)	.	.	no
C14	H17"	3.07(3)	.	.	no
C14	H13	2.13(2)	.	.	no
C114	C15	2.887(3)	.	.	no
C114	N11	3.167(3)	.	.	no
C114	C14	3.256(3)	.	.	no
C14	H17	2.84(3)	.	.	no
C15	H114	2.84(2)	.	.	no
C115	C211	3.582(4)	.	2_545	no
C115	C126	3.593(4)	.	.	no
C115	F22	3.182(3)	.	2_545	no
C15	H14	2.11(3)	.	.	no
C15	H11	2.08(2)	.	.	no
C116	F215	3.326(3)	.	.	no
C17	H14	2.80(2)	.	.	no
C17	H114	2.83(2)	.	.	no
C18	H11	2.91(2)	.	.	no
C18	H110	2.58(2)	.	.	no
C121	C210	3.512(3)	.	.	no
C121	C29	3.496(3)	.	.	no
C22	H125'	3.06(2)	.	1_655	no
C122	C129	3.576(3)	.	3_555	no
C122	F214	3.224(3)	.	.	no
C123	F217	3.261(3)	.	3_655	no
C25	H115'	2.91(3)	.	1_655	no
C125	C128	3.446(4)	.	.	no
C125	C11	3.546(4)	.	.	no
C126	C115	3.593(4)	.	.	no
C126	F218	3.325(3)	.	1_455	no
C126	C111	3.419(4)	.	.	no
C126	F212	3.303(3)	.	1_455	no
C128	C125	3.446(4)	.	.	no
C128	N11	3.417(3)	.	.	no
C128	F221	3.020(3)	.	4_454	no
C129	N11	3.166(3)	.	.	no
C129	C122	3.576(3)	.	3_555	no
C110	H124	2.87(2)	.	.	no
C210	C111	3.510(3)	.	2_555	no
C210	C121	3.512(3)	.	.	no
C110	H18'	2.91(2)	.	.	no
C110	H18"	2.85(2)	.	.	no
C210	C110	3.499(3)	.	2_555	no
C211	C115	3.582(4)	.	2_555	no
C111	H126"	2.85(2)	.	.	no
C212	C22	3.419(3)	.	.	no
C212	F22	2.830(2)	.	.	no
C112	H126"	2.83(2)	.	.	no
C213	F212	3.131(2)	.	.	no
C213	F26	2.951(2)	.	.	no
C213	F224	2.846(2)	.	.	no
C214	C224	3.328(3)	.	.	no
C114	H17	2.76(3)	.	.	no
C214	F224	2.764(2)	.	.	no
C216	C12	3.376(3)	.	2_545	no
C216	C11	3.383(3)	.	2_545	no
C217	C11	3.308(3)	.	2_545	no
C117	H13	2.96(2)	.	.	no
C217	C12	3.283(3)	.	2_545	no
C117	H129	3.09(3)	.	.	no

C118	H116"	2.99(4)	.	3_555	no
C118	H128"	2.90(3)	.	.	no
C218	C12	3.472(3)	.	2_545	no
C218	C26	3.398(3)	.	.	no
C218	F212	3.126(2)	.	.	no
C218	F26	3.063(2)	.	.	no
C219	F214	2.912(2)	.	.	no
C219	F26	3.096(2)	.	.	no
C219	F28	2.815(2)	.	.	no
C220	F28	2.749(2)	.	.	no
C220	C28	3.326(3)	.	.	no
C221	C223	3.345(3)	.	3_656	no
C221	C222	3.402(3)	.	3_656	no
C222	C223	3.406(3)	.	3_656	no
C222	C222	3.185(3)	.	3_656	no
C222	C221	3.402(3)	.	3_656	no
C122	H129'	2.94(3)	.	3_555	no
C222	C17	3.476(3)	.	.	no
C223	C17	3.275(3)	.	.	no
C223	F221	3.367(3)	.	3_656	no
C223	C221	3.345(3)	.	3_656	no
C223	C222	3.406(3)	.	3_656	no
C124	H11	2.87(2)	.	.	no
C224	F26	3.099(2)	.	.	no
C224	C214	3.328(3)	.	.	no
C224	F214	2.926(2)	.	.	no
C125	H11	3.08(2)	.	.	no
C125	H127	2.73(2)	.	.	no
C125	H128	2.88(3)	.	.	no
C126	H127	2.46(2)	.	.	no
C127	H125"	2.76(3)	.	.	no
C127	H126	2.84(3)	.	.	no
C127	H126"	3.06(2)	.	.	no
C128	H118	3.05(3)	.	.	no
C128	H125"	3.00(3)	.	.	no
C211	H115"	2.93(3)	.	2_555	no
C214	H122	3.02(2)	.	.	no
C218	H12	3.07(2)	.	2_545	no
C222	H17"	2.85(3)	.	.	no
C223	H17'	3.04(3)	.	.	no
C223	H17"	3.04(3)	.	.	no
H115'	C25	2.91(3)	.	1_455	no
H115"	F211	2.70(4)	.	2_545	no
H115"	C211	2.93(3)	.	2_545	no
H116'	V1	3.51(3)	.	.	no
H116'	H114	2.54(4)	.	.	no
H116'	N11	2.86(3)	.	.	no
H116'	F215	2.87(3)	.	.	no
H116"	H112	2.38(4)	.	.	no
H116"	C118	2.99(4)	.	3_555	no
H123"	H121	2.37(5)	.	.	no
H125'	H126'	2.55(3)	.	.	no
H125'	F22	2.71(2)	.	1_455	no
H125'	C22	3.06(2)	.	1_455	no
H125"	H127	2.25(3)	.	.	no
H125"	C127	2.76(3)	.	.	no
H125"	C128	3.00(3)	.	.	no
H125"	H126	2.48(3)	.	.	no
H125"	H128	2.40(4)	.	.	no
H126'	F218	2.68(3)	.	1_455	no
H126'	H125'	2.55(3)	.	.	no

H126"	C127	3.06(2)	.	.	no
H126"	C112	2.83(2)	.	.	no
H126"	C111	2.85(2)	.	.	no
H11	C124	2.87(2)	.	.	no
H11	C18	2.91(2)	.	.	no
H11	H18"	2.25(3)	.	.	no
H11	H124	2.17(3)	.	.	no
H11	C125	3.08(2)	.	.	no
H11	H125	2.59(4)	.	.	no
H128'	F221	2.80(3)	.	4_454	no
H128'	H129'	2.47(4)	.	.	no
H12	H125	2.40(4)	.	.	no
H12	F26	2.46(2)	.	2_555	no
H12	F224	2.85(2)	.	2_555	no
H12	C218	3.07(2)	.	2_555	no
H128"	F221	2.64(3)	.	4_454	no
H128"	H118	2.10(4)	.	.	no
H128"	C118	2.90(3)	.	.	no
H128"	V1	3.09(2)	.	.	no
H128"	N11	2.67(3)	.	.	no
H13	F29	2.82(2)	.	.	no
H13	F224	2.38(2)	.	2_555	no
H13	C117	2.96(2)	.	.	no
H129'	H128'	2.47(4)	.	.	no
H129'	C122	2.94(3)	.	3_555	no
H14	C17	2.80(2)	.	.	no
H14	H17	2.38(4)	.	.	no
H14	F28	2.44(3)	.	.	no
H17	C114	2.76(3)	.	.	no
H17	F214	2.87(3)	.	.	no
H17	C14	2.84(3)	.	.	no
H17	H14	2.38(4)	.	.	no
H17	H114	2.26(4)	.	.	no
H17'	F223	2.76(3)	.	.	no
H17'	F210	2.75(3)	.	2_545	no
H17'	C223	3.04(3)	.	.	no
H17'	H18'	2.51(4)	.	.	no
H17"	C222	2.85(3)	.	.	no
H17"	C14	3.07(3)	.	.	no
H17"	C223	3.04(3)	.	.	no
H17"	H18	2.42(4)	.	.	no
H18	H17"	2.42(4)	.	.	no
H18'	C110	2.91(2)	.	.	no
H18'	H17'	2.51(4)	.	.	no
H18'	H110	2.44(3)	.	.	no
H18'	F24	2.86(2)	.	3_656	no
H18"	C110	2.85(2)	.	.	no
H18"	F24	2.71(3)	.	1_455	no
H18"	C11	2.68(2)	.	.	no
H18"	H11	2.25(3)	.	.	no
H18"	H110	2.40(3)	.	.	no
H110	H18"	2.40(3)	.	.	no
H110	F24	2.65(2)	.	1_455	no
H110	C18	2.58(2)	.	.	no
H110	H18'	2.44(3)	.	.	no
H112	H115	2.42(4)	.	.	no
H112	F22	2.81(2)	.	2_545	no
H112	H116"	2.38(4)	.	.	no
H114	C17	2.83(2)	.	.	no
H114	H17	2.26(4)	.	.	no
H114	H116'	2.54(4)	.	.	no

H115	H112	2.42(4)	.	.	no
H115	F22	2.47(3)	.	2_545	no
H118	H128"	2.10(4)	.	.	no
H118	C128	3.05(3)	.	.	no
H118	F221	2.59(3)	.	4_454	no
H121	H123"	2.37(5)	.	.	no
H122	C214	3.02(2)	.	.	no
H122	F214	2.38(2)	.	.	no
H122	F215	2.75(2)	.	.	no
H123	F210	2.81(4)	.	.	no
H123	F23	2.84(4)	.	4_454	no
H124	C11	2.64(2)	.	.	no
H124	C110	2.87(2)	.	.	no
H124	H11	2.17(3)	.	.	no
H125	C11	2.97(3)	.	.	no
H125	C12	2.89(3)	.	.	no
H125	H11	2.59(4)	.	.	no
H125	H12	2.40(4)	.	.	no
H126	F212	2.87(3)	.	1_455	no
H126	H127	2.10(3)	.	.	no
H126	C127	2.84(3)	.	.	no
H126	H125"	2.48(3)	.	.	no
H127	H126	2.10(3)	.	.	no
H127	C125	2.73(2)	.	.	no
H127	H125"	2.25(3)	.	.	no
H127	C126	2.46(2)	.	.	no
H128	F25	2.83(3)	.	2_555	no
H128	F26	2.81(3)	.	2_555	no
H128	H125"	2.40(4)	.	.	no
H128	C125	2.88(3)	.	.	no
H129	C117	3.09(3)	.	.	no
H129	V1	3.25(2)	.	.	no
H129	N11	2.50(3)	.	.	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)

#

C12	H12	F26	0.92(2)	2.46(2)	3.352(3)	164.8(19)	2_555	yes
C13	H13	F224	0.96(2)	2.38(2)	2.980(2)	119.7(17)	2_555	yes
C14	H14	F28	0.94(3)	2.44(3)	3.236(3)	141.9(19)	.	yes
C115	H115	F22	0.95(3)	2.47(3)	3.182(3)	131(3)	2_545	yes
C122	H122	F214	0.97(2)	2.38(2)	3.224(3)	144.4(18)	.	yes
C129	H129	N11	0.95(3)	2.50(3)	3.166(3)	127.4(19)	.	yes

Loop Mechanism for Extra Tables(s)

#loop_

#_publ_manuscript_incl_extra_item

#'_geom_extra_tableA_col_1'

#'_geom_extra_tableA_col_2'

#'_geom_extra_tableA_col_3'

```
#'_geom_extra_table_head_A'  
#'_geom_table_footnote_A'  
#'_geom_extra_tableB_col_1'  
#'_geom_extra_tableB_col_2'  
#'_geom_extra_tableB_col_3'  
#'_geom_extra_table_head_B'  
#'_geom_table_footnote_B'
```

```
#  
#loop_  
#_geom_extra_tableA_col_1  
#_geom_extra_tableA_col_2  
#_geom_extra_tableA_col_3  
# ? ? ?
```

```
#  
#loop_  
#_geom_extra_tableB_col_1  
#_geom_extra_tableB_col_2  
#_geom_extra_tableB_col_3  
# ? ? ?
```

```
#  
#_geom_table_footnote_A  
#;  
# ?  
#;
```

```
#  
#_geom_table_footnote_B  
#;  
# ?  
#;
```

```
#  
#_geom_table_footnote_A  
#;  
# ?  
#;
```

```
#  
#_geom_table_footnote_B  
#;  
# ?  
#;
```

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