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Strategies for the synthesis of lanthanum dialkyl complexes with monoanionic ancillary ligands

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SHELXL97-2 & Manual Editing
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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.
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_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 'Organo Metallica'
Publication choice 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 : 2007-08-29 15:34:47

Consider this CIF submission for deposition of the fourth
X-ray structure of a manuscript to be submitted to : Organo Metallica
(Our Compound_Identification_Code : Q1077)

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2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_printers_final        ?
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_journal_page_last                  ?

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# 3. TITLE AND AUTHOR LIST

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;
_publ_section_title_footnote
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;

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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
;
?
;
_publ_section_abstract
;
?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
The asymmetric unit consists of four moieties: a cationic La-complex,
a tetraphenylborate anion and a disordered THF solvate molecule.
;
_publ_section_exptl_prep
;
?
;
_publ_section_exptl_refinement
;
The positional and anisotropic displacement parameters for the
non-hydrogen atoms were refined. A few atoms showed unrealistic
displacement parameters when allowed to vary anisotropically,
suggesting dynamic disorder (dynamic means that the smeared
electron density is due to fluctuations of the atomic positions
within each unit cell; the disorder is compensated by the larger
the displacement parameters), especially the THF solvate molecule.
The hydrogen atoms were generated by geometrical considerations,
constrained to idealized geometries, and allowed to ride on their
carrier atoms with an isotropic displacement parameter related
to the equivalent displacement parameter of their carrier atoms.
;

# Insert blank lines between references

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

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

```

Laboratory, University of Nijmegen, The Netherlands.

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Bruker, (2000). SMART, SAINTPLUS and XPREP.
Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

Hahn, T. (1983) Ed. International Tables for Crystallography,
Volume A, Space-group symmetry, Kluwer Academic Publishers,
Dordrecht, The Netherlands.

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Multi-Scan Absorption Correction Program.
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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

'C48 H74 La N2 O3, C24 H20 B, C4 H8 O'

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'

_chemical_formula_structural ?

_chemical_formula_sum

'C76 H102 B La N2 O4'

_chemical_formula_iupac ?

_chemical_formula_weight 1257.37
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
O O 0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
La La -0.2871 2.4523
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B B 0.0013 0.0007
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H H 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

6. CRYSTAL DATA

_symmetry_cell_setting Monoclinic
_symmetry_space_group_name_Hall '-P 2ybc'
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14

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

_cell_length_a 21.148(1)
_cell_length_b 17.242(1)
_cell_length_c 18.497(1)
_cell_angle_alpha 90
_cell_angle_beta 92.309(1)
_cell_angle_gamma 90
_cell_volume 6739.2(6)
_cell_formula_units_Z 4

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 6603
_cell_measurement_theta_min 2.36
_cell_measurement_theta_max 28.30
_cell_special_details

;

The final unit cell was obtained from the xyz centroids of
6603 reflections after integration using the SAINT software
package (Bruker, 2000).

;

_exptl_crystal_description 'block'
_exptl_crystal_colour 'yellow'

```

_exptl_crystal_size_max      0.35
_exptl_crystal_size_mid     0.24
_exptl_crystal_size_min     0.19
_exptl_crystal_size_rad     ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.239
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000        2664
_exptl_absorpt_coefficient_mu 0.683
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min 0.7794
_exptl_absorpt_correction_T_max 0.8811

```

#=====

7. EXPERIMENTAL DATA

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; ?
;
_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 ?
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_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            53027
_diffn_reflns_av_R_equivalents  0.0532
_diffn_reflns_av_sigmaI/netI    0.0519
_diffn_reflns_limit_h_min       -26
_diffn_reflns_limit_h_max       26
_diffn_reflns_limit_k_min       -21
_diffn_reflns_limit_k_max       21

```

```

_diffrn_reflms_limit_l_min      -23
_diffrn_reflms_limit_l_max      23
_diffrn_reflms_theta_min        2.26
_diffrn_reflms_theta_max        26.37
_diffrn_measured_fraction_theta_max  0.998
_diffrn_reflms_theta_full       25.00
_diffrn_measured_fraction_theta_full  0.999

_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            13749
_reflms_number_gt               11237
_reflms_threshold_expression     I>2\s(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, 2005)
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/[\s^2*(Fo^2)+(0.0334P)^2+26.0070P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary     heavy
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    constr

```



```

_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?

_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          13749
_refine_ls_number_parameters      768
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0713
_refine_ls_R_factor_gt            0.0575
_refine_ls_wR_factor_ref          0.1341
_refine_ls_wR_factor_gt          0.1290
_refine_ls_goodness_of_fit_ref    1.147
_refine_ls_restrained_S_all       1.147
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          2.234
_refine_diff_density_min          -1.913
_refine_diff_density_rms          0.103

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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
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_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
La1 La Uani 0.23619(1) 0.51272(1) 0.75132(1) 1.000 0.0165(1) . .
O11 O Uani 0.29063(14) 0.51660(18) 0.62892(16) 1.000 0.0239(9) . .
O12 O Uani 0.33325(14) 0.42384(18) 0.76335(17) 1.000 0.0240(9) . .
O13 O Uani 0.27424(15) 0.51103(19) 0.88440(16) 1.000 0.0266(9) . .
N11 N Uani 0.13471(16) 0.4845(2) 0.68324(18) 1.000 0.0183(10) . .
N12 N Uani 0.12726(16) 0.4869(2) 0.80222(18) 1.000 0.0175(10) . .
C11 C Uani 0.12477(18) 0.4596(3) 0.6104(2) 1.000 0.0173(11) . .
C12 C Uani 0.1185(2) 0.5137(3) 0.5535(2) 1.000 0.0237(12) . .
C13 C Uani 0.1187(2) 0.4859(3) 0.4825(2) 1.000 0.0297(16) . .
C14 C Uani 0.1256(2) 0.4088(3) 0.4669(3) 1.000 0.0320(16) . .
C15 C Uani 0.1323(2) 0.3557(3) 0.5233(3) 1.000 0.0271(14) . .
C16 C Uani 0.13196(19) 0.3794(3) 0.5954(2) 1.000 0.0207(12) . .
C17 C Uani 0.1153(2) 0.6011(3) 0.5667(2) 1.000 0.0234(12) . .
C18 C Uani 0.1784(2) 0.6394(3) 0.5494(3) 1.000 0.0321(17) . .
C19 C Uani 0.0619(2) 0.6406(3) 0.5227(3) 1.000 0.0314(17) . .
C110 C Uani 0.1430(2) 0.3202(3) 0.6553(2) 1.000 0.0226(12) . .
C111 C Uani 0.1128(3) 0.2409(3) 0.6391(3) 1.000 0.0365(17) . .
C112 C Uani 0.2135(2) 0.3096(3) 0.6734(3) 1.000 0.0276(14) . .
C113 C Uani 0.09590(18) 0.4794(2) 0.7386(2) 1.000 0.0149(11) . .

```

| | | | | | | | | |
|------|---|------|-------------|-----------|-----------|-------|------------|-------|
| C114 | C | Uani | 0.02233(19) | 0.4745(3) | 0.7269(2) | 1.000 | 0.0200(12) | . . . |
| C115 | C | Uani | 0.0016(2) | 0.5447(3) | 0.6813(3) | 1.000 | 0.0307(16) | . . . |
| C116 | C | Uani | 0.0010(2) | 0.4002(3) | 0.6868(3) | 1.000 | 0.0297(16) | . . . |
| C117 | C | Uani | -0.0150(2) | 0.4780(3) | 0.7966(2) | 1.000 | 0.0243(14) | . . . |
| C118 | C | Uani | 0.10502(18) | 0.4822(3) | 0.8737(2) | 1.000 | 0.0196(11) | . . . |
| C119 | C | Uani | 0.0938(2) | 0.4083(3) | 0.9045(3) | 1.000 | 0.0257(14) | . . . |
| C120 | C | Uani | 0.0816(2) | 0.4034(3) | 0.9774(3) | 1.000 | 0.0336(16) | . . . |
| C121 | C | Uani | 0.0794(2) | 0.4688(3) | 1.0200(3) | 1.000 | 0.0380(18) | . . . |
| C122 | C | Uani | 0.0886(2) | 0.5401(3) | 0.9904(3) | 1.000 | 0.0334(14) | . . . |
| C123 | C | Uani | 0.1022(2) | 0.5489(3) | 0.9164(2) | 1.000 | 0.0254(14) | . . . |
| C124 | C | Uani | 0.0965(2) | 0.3351(3) | 0.8606(3) | 1.000 | 0.0284(14) | . . . |
| C125 | C | Uani | 0.0464(3) | 0.2743(3) | 0.8784(3) | 1.000 | 0.0419(19) | . . . |
| C126 | C | Uani | 0.1625(2) | 0.2997(3) | 0.8663(3) | 1.000 | 0.0361(17) | . . . |
| C127 | C | Uani | 0.1126(2) | 0.6286(3) | 0.8862(3) | 1.000 | 0.0287(16) | . . . |
| C128 | C | Uani | 0.1624(3) | 0.6748(3) | 0.9307(3) | 1.000 | 0.0378(17) | . . . |
| C129 | C | Uani | 0.0505(2) | 0.6753(3) | 0.8804(3) | 1.000 | 0.0375(17) | . . . |
| C130 | C | Uani | 0.2553(2) | 0.6554(3) | 0.7645(3) | 1.000 | 0.0300(14) | . . . |
| C131 | C | Uani | 0.2306(2) | 0.7226(3) | 0.7229(2) | 1.000 | 0.0267(14) | . . . |
| C132 | C | Uani | 0.2695(3) | 0.7656(3) | 0.6798(3) | 1.000 | 0.0346(17) | . . . |
| C133 | C | Uani | 0.2472(3) | 0.8284(3) | 0.6396(3) | 1.000 | 0.0414(19) | . . . |
| C134 | C | Uani | 0.1851(3) | 0.8514(3) | 0.6417(3) | 1.000 | 0.0430(19) | . . . |
| C135 | C | Uani | 0.1445(3) | 0.8087(3) | 0.6847(3) | 1.000 | 0.0426(17) | . . . |
| C136 | C | Uani | 0.1671(2) | 0.7457(3) | 0.7240(3) | 1.000 | 0.0326(17) | . . . |
| C137 | C | Uani | 0.3384(2) | 0.5751(3) | 0.6126(3) | 1.000 | 0.0290(16) | . . . |
| C138 | C | Uani | 0.3690(3) | 0.5439(3) | 0.5469(3) | 1.000 | 0.0406(17) | . . . |
| C139 | C | Uani | 0.3184(3) | 0.4983(4) | 0.5088(3) | 1.000 | 0.0497(19) | . . . |
| C140 | C | Uani | 0.2857(3) | 0.4609(3) | 0.5713(3) | 1.000 | 0.0420(19) | . . . |
| C141 | C | Uani | 0.3381(2) | 0.3599(3) | 0.8147(3) | 1.000 | 0.0273(16) | . . . |
| C142 | C | Uani | 0.3770(2) | 0.3000(3) | 0.7773(3) | 1.000 | 0.0358(17) | . . . |
| C143 | C | Uani | 0.4238(3) | 0.3495(3) | 0.7375(3) | 1.000 | 0.0425(17) | . . . |
| C144 | C | Uani | 0.3927(3) | 0.4251(4) | 0.7286(4) | 1.000 | 0.073(3) | . . . |
| C145 | C | Uani | 0.2561(2) | 0.4689(3) | 0.9494(3) | 1.000 | 0.0325(16) | . . . |
| C146 | C | Uani | 0.2892(3) | 0.5102(4) | 1.0104(3) | 1.000 | 0.049(2) | . . . |
| C147 | C | Uani | 0.3498(3) | 0.5355(4) | 0.9794(3) | 1.000 | 0.050(2) | . . . |
| C148 | C | Uani | 0.3328(2) | 0.5536(3) | 0.9012(3) | 1.000 | 0.0349(17) | . . . |

| | | | | | | | | |
|--------|---|------|----------|---------|---------|-------|--------|-------|
| H13 | H | Uiso | 0.11377 | 0.52181 | 0.44375 | 1.000 | 0.0355 | . . . |
| H14 | H | Uiso | 0.12586 | 0.39172 | 0.41806 | 1.000 | 0.0384 | . . . |
| H15 | H | Uiso | 0.13721 | 0.30226 | 0.51250 | 1.000 | 0.0325 | . . . |
| H17 | H | Uiso | 0.10787 | 0.60966 | 0.61912 | 1.000 | 0.0281 | . . . |
| H18 | H | Uiso | 0.21254 | 0.61635 | 0.57966 | 1.000 | 0.0480 | . . . |
| H18' | H | Uiso | 0.17608 | 0.69514 | 0.55910 | 1.000 | 0.0480 | . . . |
| H18'' | H | Uiso | 0.18690 | 0.63107 | 0.49824 | 1.000 | 0.0480 | . . . |
| H19 | H | Uiso | 0.06995 | 0.63644 | 0.47099 | 1.000 | 0.0469 | . . . |
| H19' | H | Uiso | 0.05977 | 0.69541 | 0.53631 | 1.000 | 0.0469 | . . . |
| H19'' | H | Uiso | 0.02160 | 0.61528 | 0.53236 | 1.000 | 0.0469 | . . . |
| H110 | H | Uiso | 0.12331 | 0.34117 | 0.69953 | 1.000 | 0.0270 | . . . |
| H111 | H | Uiso | 0.06836 | 0.24798 | 0.62354 | 1.000 | 0.0546 | . . . |
| H111' | H | Uiso | 0.11537 | 0.20888 | 0.68291 | 1.000 | 0.0546 | . . . |
| H111'' | H | Uiso | 0.13548 | 0.21525 | 0.60063 | 1.000 | 0.0546 | . . . |
| H112 | H | Uiso | 0.23475 | 0.29222 | 0.63016 | 1.000 | 0.0415 | . . . |
| H112' | H | Uiso | 0.21929 | 0.27065 | 0.71172 | 1.000 | 0.0415 | . . . |
| H112'' | H | Uiso | 0.23177 | 0.35901 | 0.69000 | 1.000 | 0.0415 | . . . |
| H115 | H | Uiso | -0.04472 | 0.54743 | 0.67820 | 1.000 | 0.0460 | . . . |
| H115' | H | Uiso | 0.01763 | 0.53957 | 0.63252 | 1.000 | 0.0460 | . . . |
| H115'' | H | Uiso | 0.01860 | 0.59213 | 0.70386 | 1.000 | 0.0460 | . . . |
| H116 | H | Uiso | -0.04512 | 0.40072 | 0.67905 | 1.000 | 0.0447 | . . . |
| H116' | H | Uiso | 0.01354 | 0.35477 | 0.71582 | 1.000 | 0.0447 | . . . |
| H116'' | H | Uiso | 0.02098 | 0.39774 | 0.63995 | 1.000 | 0.0447 | . . . |
| H117 | H | Uiso | -0.00445 | 0.52596 | 0.82274 | 1.000 | 0.0360 | . . . |

H117' H Uiso -0.00374 0.43327 0.82721 1.000 0.0360 . .
H117" H Uiso -0.06043 0.47686 0.78410 1.000 0.0360 . .
H120 H Uiso 0.07450 0.35406 0.99844 1.000 0.0405 . .
H121 H Uiso 0.07157 0.46413 1.07003 1.000 0.0457 . .
H122 H Uiso 0.08581 0.58493 1.02002 1.000 0.0399 . .
H124 H Uiso 0.08845 0.35019 0.80881 1.000 0.0338 . .
H125 H Uiso 0.05539 0.25383 0.92715 1.000 0.0627 . .
H125' H Uiso 0.04753 0.23177 0.84323 1.000 0.0627 . .
H125" H Uiso 0.00440 0.29829 0.87607 1.000 0.0627 . .
H126 H Uiso 0.19352 0.33773 0.85057 1.000 0.0543 . .
H126' H Uiso 0.16392 0.25358 0.83549 1.000 0.0543 . .
H126" H Uiso 0.17258 0.28503 0.91669 1.000 0.0543 . .
H127 H Uiso 0.12828 0.62239 0.83620 1.000 0.0345 . .
H128 H Uiso 0.14561 0.68795 0.97780 1.000 0.0567 . .
H128' H Uiso 0.17253 0.72250 0.90486 1.000 0.0567 . .
H128" H Uiso 0.20073 0.64340 0.93795 1.000 0.0567 . .
H129 H Uiso 0.01877 0.64622 0.85150 1.000 0.0559 . .
H129' H Uiso 0.05829 0.72529 0.85714 1.000 0.0559 . .
H129" H Uiso 0.03508 0.68419 0.92897 1.000 0.0559 . .
H130 H Uiso 0.24454 0.66687 0.81496 1.000 0.0357 . .
H130' H Uiso 0.30180 0.66076 0.76326 1.000 0.0357 . .
H132 H Uiso 0.31287 0.75161 0.67776 1.000 0.0417 . .
H133 H Uiso 0.27523 0.85602 0.61004 1.000 0.0497 . .
H134 H Uiso 0.17006 0.89497 0.61478 1.000 0.0513 . .
H135 H Uiso 0.10131 0.82323 0.68675 1.000 0.0507 . .
H136 H Uiso 0.13881 0.71732 0.75262 1.000 0.0393 . .
H137 H Uiso 0.36968 0.58089 0.65347 1.000 0.0347 . .
H137' H Uiso 0.31835 0.62602 0.60230 1.000 0.0347 . .
H138 H Uiso 0.38367 0.58663 0.51595 1.000 0.0488 . .
H138' H Uiso 0.40559 0.51046 0.56077 1.000 0.0488 . .
H139 H Uiso 0.33626 0.45890 0.47647 1.000 0.0595 . .
H139' H Uiso 0.28911 0.53231 0.48018 1.000 0.0595 . .
H140 H Uiso 0.24080 0.44985 0.55798 1.000 0.0501 . .
H140' H Uiso 0.30693 0.41178 0.58574 1.000 0.0501 . .
H141 H Uiso 0.29573 0.33926 0.82500 1.000 0.0327 . .
H141' H Uiso 0.35944 0.37670 0.86071 1.000 0.0327 . .
H142 H Uiso 0.35046 0.26852 0.74318 1.000 0.0429 . .
H142' H Uiso 0.39899 0.26519 0.81270 1.000 0.0429 . .
H143 H Uiso 0.46418 0.35462 0.76619 1.000 0.0511 . .
H143' H Uiso 0.43261 0.32654 0.68993 1.000 0.0511 . .
H144 H Uiso 0.42009 0.46625 0.75025 1.000 0.0871 . .
H144' H Uiso 0.38563 0.43667 0.67647 1.000 0.0871 . .
H145 H Uiso 0.26996 0.41407 0.94749 1.000 0.0388 . .
H145' H Uiso 0.20971 0.47034 0.95440 1.000 0.0388 . .
H146 H Uiso 0.29701 0.47518 1.05223 1.000 0.0592 . .
H146' H Uiso 0.26422 0.55536 1.02604 1.000 0.0592 . .
H147 H Uiso 0.38178 0.49359 0.98321 1.000 0.0601 . .
H147' H Uiso 0.36677 0.58201 1.00479 1.000 0.0601 . .
H148 H Uiso 0.32621 0.61000 0.89431 1.000 0.0419 . .
H148' H Uiso 0.36676 0.53631 0.86958 1.000 0.0419 . .

C21 C Uani 0.4938(2) 0.3261(3) 0.4096(2) 1.000 0.0214(12) . .
C22 C Uani 0.4757(2) 0.3971(3) 0.4400(3) 1.000 0.0260(14) . .
C23 C Uani 0.4667(2) 0.4641(3) 0.4005(3) 1.000 0.0292(16) . .
C24 C Uani 0.4758(2) 0.4640(3) 0.3267(3) 1.000 0.0272(14) . .
C25 C Uani 0.4933(2) 0.3954(3) 0.2940(3) 1.000 0.0267(14) . .
C26 C Uani 0.5014(2) 0.3280(3) 0.3349(3) 1.000 0.0240(12) . .
C27 C Uani 0.4362(2) 0.2344(3) 0.5042(3) 1.000 0.0284(14) . .
C28 C Uani 0.4353(3) 0.1916(3) 0.5692(3) 1.000 0.0423(19) . .
C29 C Uani 0.3791(3) 0.1719(3) 0.6012(4) 1.000 0.063(3) . .

C210 C Uani 0.3222(3) 0.1950(3) 0.5700(4) 1.000 0.066(3) . .
C211 C Uani 0.3209(3) 0.2388(3) 0.5081(4) 1.000 0.054(2) . .
C212 C Uani 0.3772(2) 0.2577(3) 0.4763(3) 1.000 0.0365(17) . .
C213 C Uani 0.5214(2) 0.1701(3) 0.4203(2) 1.000 0.0221(12) . .
C214 C Uani 0.5704(2) 0.1672(3) 0.3703(2) 1.000 0.0264(14) . .
C215 C Uani 0.5898(2) 0.0990(3) 0.3376(2) 1.000 0.0314(16) . .
C216 C Uani 0.5604(3) 0.0299(3) 0.3529(3) 1.000 0.0344(16) . .
C217 C Uani 0.5115(2) 0.0291(3) 0.4002(3) 1.000 0.0294(17) . .
C218 C Uani 0.4928(2) 0.0979(3) 0.4325(2) 1.000 0.0231(12) . .
C219 C Uani 0.5605(2) 0.2707(3) 0.5230(2) 1.000 0.0234(12) . .
C220 C Uani 0.6247(2) 0.2551(3) 0.5132(3) 1.000 0.0295(16) . .
C221 C Uani 0.6725(3) 0.2771(3) 0.5627(3) 1.000 0.0450(19) . .
C222 C Uani 0.6586(3) 0.3150(3) 0.6258(3) 1.000 0.052(2) . .
C223 C Uani 0.5964(3) 0.3321(3) 0.6375(3) 1.000 0.050(2) . .
C224 C Uani 0.5485(3) 0.3107(3) 0.5871(3) 1.000 0.0334(16) . .
B2 B Uani 0.5028(2) 0.2498(3) 0.4634(3) 1.000 0.0199(12) . .

H22 H Uiso 0.46929 0.39887 0.49054 1.000 0.0312 . .
H23 H Uiso 0.45435 0.51041 0.42381 1.000 0.0352 . .
H24 H Uiso 0.47013 0.51004 0.29902 1.000 0.0328 . .
H25 H Uiso 0.49978 0.39430 0.24353 1.000 0.0325 . .
H26 H Uiso 0.51248 0.28142 0.31100 1.000 0.0290 . .
H28 H Uiso 0.47432 0.17586 0.59190 1.000 0.0507 . .
H29 H Uiso 0.38013 0.14249 0.64459 1.000 0.0748 . .
H210 H Uiso 0.28376 0.18060 0.59125 1.000 0.0797 . .
H211 H Uiso 0.28166 0.25612 0.48702 1.000 0.0639 . .
H212 H Uiso 0.37538 0.28803 0.43345 1.000 0.0437 . .
H214 H Uiso 0.59101 0.21418 0.35860 1.000 0.0318 . .
H215 H Uiso 0.62317 0.10016 0.30482 1.000 0.0373 . .
H216 H Uiso 0.57376 -0.01691 0.33110 1.000 0.0408 . .
H217 H Uiso 0.49072 -0.01818 0.41063 1.000 0.0352 . .
H218 H Uiso 0.45884 0.09589 0.46453 1.000 0.0275 . .
H220 H Uiso 0.63595 0.22827 0.47078 1.000 0.0351 . .
H221 H Uiso 0.71530 0.26592 0.55294 1.000 0.0538 . .
H222 H Uiso 0.69120 0.32898 0.66016 1.000 0.0626 . .
H223 H Uiso 0.58576 0.35874 0.68029 1.000 0.0602 . .
H224 H Uiso 0.50603 0.32375 0.59666 1.000 0.0401 . .

O31 O Uani 0.2065(4) 0.3805(4) 0.2856(4) 1.000 0.128(4) . .
C31 C Uani 0.2019(4) 0.4431(6) 0.2426(6) 1.000 0.103(4) . .
C32 C Uani 0.2646(7) 0.4761(9) 0.2471(10) 1.000 0.220(10) . .
C33 C Uani 0.2978(4) 0.4451(11) 0.3016(6) 1.000 0.160(7) . .
C34 C Uani 0.2626(6) 0.3831(6) 0.3297(6) 1.000 0.112(5) . .

H31 H Uiso 0.17027 0.48024 0.26033 1.000 0.1236 . .
H31' H Uiso 0.18970 0.42824 0.19229 1.000 0.1236 . .
H32 H Uiso 0.28607 0.46619 0.20134 1.000 0.2644 . .
H32' H Uiso 0.26178 0.53288 0.25389 1.000 0.2644 . .
H33 H Uiso 0.30637 0.48450 0.33969 1.000 0.1941 . .
H33' H Uiso 0.33882 0.42579 0.28491 1.000 0.1941 . .
H34 H Uiso 0.28622 0.33375 0.32670 1.000 0.1346 . .
H34' H Uiso 0.25287 0.39287 0.38078 1.000 0.1346 . .

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

La1 0.0124(1) 0.0185(1) 0.0183(1) -0.0013(1) -0.0014(1) -0.0003(1)
O11 0.0243(16) 0.0287(16) 0.0192(15) 0.0058(13) 0.0069(12) -0.0009(13)
O12 0.0172(15) 0.0285(17) 0.0264(17) 0.0055(13) 0.0028(13) 0.0032(13)
O13 0.0247(16) 0.0350(18) 0.0195(15) -0.0028(14) -0.0058(13) 0.0019(14)
N11 0.0182(17) 0.0190(17) 0.0176(17) -0.0006(14) -0.0003(14) -0.0005(14)
N12 0.0174(17) 0.0193(17) 0.0157(16) -0.0009(14) 0.0009(14) -0.0001(14)
C11 0.0089(18) 0.029(2) 0.014(2) -0.0007(17) -0.0010(15) -0.0027(16)
C12 0.017(2) 0.034(2) 0.020(2) -0.0008(19) -0.0001(17) -0.0037(19)
C13 0.035(3) 0.038(3) 0.016(2) 0.002(2) 0.0008(19) -0.003(2)
C14 0.033(3) 0.046(3) 0.017(2) -0.008(2) 0.000(2) -0.002(2)
C15 0.024(2) 0.031(3) 0.026(2) -0.013(2) -0.0017(19) 0.0001(19)
C16 0.014(2) 0.029(2) 0.019(2) -0.0045(18) -0.0002(17) -0.0037(17)
C17 0.022(2) 0.028(2) 0.020(2) 0.0027(18) 0.0003(18) 0.0007(18)
C18 0.026(3) 0.033(3) 0.037(3) 0.008(2) -0.002(2) 0.001(2)
C19 0.026(3) 0.040(3) 0.028(3) 0.008(2) -0.002(2) 0.004(2)
C110 0.019(2) 0.024(2) 0.025(2) -0.0046(18) 0.0027(18) -0.0001(18)
C111 0.039(3) 0.027(3) 0.043(3) 0.001(2) -0.005(2) -0.011(2)
C112 0.024(2) 0.026(2) 0.033(3) -0.002(2) 0.002(2) -0.0001(19)
C113 0.0153(19) 0.0104(19) 0.019(2) 0.0010(16) -0.0009(16) 0.0006(15)
C114 0.016(2) 0.026(2) 0.018(2) 0.0006(17) -0.0004(16) 0.0008(17)
C115 0.018(2) 0.043(3) 0.031(3) 0.011(2) 0.001(2) 0.005(2)
C116 0.017(2) 0.042(3) 0.030(3) -0.008(2) 0.000(2) -0.005(2)
C117 0.016(2) 0.035(3) 0.022(2) 0.0005(19) 0.0009(17) 0.0007(19)
C118 0.0099(18) 0.035(2) 0.0138(19) 0.0004(18) 0.0000(15) 0.0026(18)
C119 0.013(2) 0.042(3) 0.022(2) 0.009(2) 0.0003(18) 0.0025(19)
C120 0.021(2) 0.054(3) 0.026(3) 0.014(2) 0.002(2) 0.004(2)
C121 0.030(3) 0.066(4) 0.018(2) 0.008(2) 0.003(2) 0.005(3)
C122 0.020(2) 0.056(3) 0.024(2) -0.012(2) -0.0001(19) 0.009(2)
C123 0.015(2) 0.040(3) 0.021(2) -0.005(2) -0.0028(18) 0.0049(19)
C124 0.023(2) 0.036(3) 0.026(2) 0.012(2) -0.002(2) -0.003(2)
C125 0.030(3) 0.040(3) 0.055(4) 0.016(3) -0.006(3) -0.007(2)
C126 0.027(3) 0.037(3) 0.045(3) 0.002(2) 0.009(2) -0.004(2)
C127 0.021(2) 0.037(3) 0.028(3) -0.011(2) -0.001(2) 0.005(2)
C128 0.032(3) 0.039(3) 0.042(3) -0.012(2) -0.004(2) 0.001(2)
C129 0.031(3) 0.037(3) 0.044(3) -0.007(2) -0.003(2) 0.010(2)
C130 0.022(2) 0.026(2) 0.042(3) 0.002(2) 0.000(2) 0.0008(19)
C131 0.033(3) 0.027(2) 0.020(2) -0.0057(19) -0.001(2) -0.005(2)
C132 0.029(3) 0.037(3) 0.038(3) 0.002(2) 0.003(2) -0.004(2)
C133 0.050(4) 0.041(3) 0.033(3) 0.010(2) -0.001(3) -0.008(3)
C134 0.059(4) 0.033(3) 0.036(3) 0.008(2) -0.012(3) 0.000(3)
C135 0.035(3) 0.045(3) 0.047(3) -0.004(3) -0.007(3) 0.011(2)
C136 0.030(3) 0.034(3) 0.034(3) -0.001(2) 0.004(2) -0.002(2)
C137 0.020(2) 0.033(3) 0.034(3) 0.003(2) 0.000(2) -0.007(2)
C138 0.040(3) 0.040(3) 0.043(3) 0.003(3) 0.015(3) -0.009(2)
C139 0.045(3) 0.066(4) 0.039(3) -0.009(3) 0.014(3) -0.010(3)
C140 0.037(3) 0.035(3) 0.056(4) -0.013(3) 0.025(3) -0.015(2)
C141 0.021(2) 0.032(3) 0.029(3) 0.007(2) 0.0038(19) 0.0040(19)
C142 0.028(3) 0.034(3) 0.046(3) 0.002(2) 0.010(2) 0.009(2)
C143 0.034(3) 0.047(3) 0.048(3) 0.002(3) 0.020(3) 0.010(2)
C144 0.027(3) 0.088(5) 0.105(6) 0.060(5) 0.032(4) 0.024(3)
C145 0.028(3) 0.047(3) 0.022(2) -0.002(2) -0.004(2) 0.006(2)
C146 0.064(4) 0.052(4) 0.031(3) -0.005(3) -0.014(3) 0.002(3)
C147 0.045(4) 0.062(4) 0.042(3) -0.015(3) -0.020(3) 0.001(3)
C148 0.027(3) 0.040(3) 0.037(3) -0.003(2) -0.008(2) -0.002(2)
C21 0.017(2) 0.026(2) 0.021(2) 0.0008(18) -0.0011(17) -0.0041(17)
C22 0.028(3) 0.027(2) 0.023(2) -0.0003(19) 0.000(2) 0.0005(19)
C23 0.028(3) 0.025(2) 0.034(3) -0.002(2) -0.006(2) 0.0044(19)

C24 0.022(2) 0.026(2) 0.033(3) 0.008(2) -0.005(2) 0.0006(19)
 C25 0.022(2) 0.033(3) 0.025(2) 0.006(2) -0.0012(19) -0.0030(19)
 C26 0.019(2) 0.026(2) 0.027(2) -0.0006(19) 0.0009(19) -0.0025(18)
 C27 0.027(2) 0.020(2) 0.039(3) -0.007(2) 0.012(2) -0.0023(19)
 C28 0.050(3) 0.023(3) 0.056(4) 0.008(2) 0.030(3) 0.007(2)
 C29 0.076(5) 0.024(3) 0.092(5) 0.007(3) 0.061(4) 0.008(3)
 C210 0.063(5) 0.022(3) 0.119(6) -0.014(3) 0.070(5) -0.011(3)
 C211 0.024(3) 0.038(3) 0.100(5) -0.032(4) 0.022(3) -0.008(2)
 C212 0.028(3) 0.030(3) 0.052(3) -0.020(2) 0.009(2) -0.002(2)
 C213 0.023(2) 0.025(2) 0.018(2) 0.0003(18) -0.0040(18) 0.0028(18)
 C214 0.026(2) 0.033(3) 0.020(2) 0.0008(19) -0.0025(19) 0.004(2)
 C215 0.032(3) 0.046(3) 0.016(2) -0.002(2) -0.003(2) 0.013(2)
 C216 0.046(3) 0.034(3) 0.022(2) -0.009(2) -0.013(2) 0.015(2)
 C217 0.036(3) 0.022(3) 0.029(3) -0.0034(19) -0.013(2) 0.002(2)
 C218 0.019(2) 0.026(2) 0.024(2) -0.0035(18) -0.0039(18) 0.0018(18)
 C219 0.030(2) 0.020(2) 0.020(2) 0.0034(17) -0.0013(19) -0.0007(18)
 C220 0.030(3) 0.022(2) 0.036(3) 0.000(2) -0.004(2) -0.0007(19)
 C221 0.031(3) 0.034(3) 0.068(4) -0.003(3) -0.022(3) 0.004(2)
 C222 0.067(4) 0.032(3) 0.055(4) -0.011(3) -0.038(3) 0.005(3)
 C223 0.075(5) 0.040(3) 0.034(3) -0.008(3) -0.022(3) 0.014(3)
 C224 0.047(3) 0.032(3) 0.021(2) 0.002(2) -0.002(2) 0.008(2)
 B2 0.019(2) 0.021(2) 0.020(2) 0.0005(19) 0.004(2) -0.0003(19)
 O31 0.183(8) 0.089(5) 0.105(5) 0.031(4) -0.081(5) -0.074(5)
 C31 0.067(6) 0.098(7) 0.140(9) 0.045(7) -0.039(6) -0.021(5)
 C32 0.160(14) 0.179(15) 0.31(2) 0.164(16) -0.112(15) -0.079(12)
 C33 0.054(6) 0.34(2) 0.085(7) 0.065(10) -0.019(5) -0.081(9)
 C34 0.140(10) 0.078(7) 0.114(9) 0.005(6) -0.045(8) 0.015(6)

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10. MOLECULAR GEOMETRY

_geom_special_details

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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

| | | | | | |
|-----|------|-----------|---|---|-----|
| La1 | O11 | 2.582(3) | . | . | yes |
| La1 | O12 | 2.564(3) | . | . | yes |
| La1 | O13 | 2.559(3) | . | . | yes |
| La1 | N11 | 2.492(3) | . | . | yes |
| La1 | N12 | 2.563(3) | . | . | yes |
| La1 | C130 | 2.503(5) | . | . | yes |
| O11 | C137 | 1.468(6) | . | . | yes |
| O11 | C140 | 1.435(6) | . | . | yes |
| O12 | C141 | 1.456(6) | . | . | yes |
| O12 | C144 | 1.435(7) | . | . | yes |
| O13 | C145 | 1.469(6) | . | . | yes |
| O13 | C148 | 1.462(6) | . | . | yes |
| O31 | C34 | 1.413(15) | . | . | yes |

| | | | | | |
|------|-------|------------|---|---|-----|
| O31 | C31 | 1.342 (13) | . | . | yes |
| N11 | C113 | 1.341 (5) | . | . | yes |
| N11 | C11 | 1.422 (5) | . | . | yes |
| N12 | C113 | 1.334 (5) | . | . | yes |
| N12 | C118 | 1.423 (5) | . | . | yes |
| C11 | C12 | 1.409 (6) | . | . | no |
| C11 | C16 | 1.420 (7) | . | . | no |
| C12 | C17 | 1.529 (7) | . | . | no |
| C12 | C13 | 1.398 (6) | . | . | no |
| C13 | C14 | 1.369 (7) | . | . | no |
| C14 | C15 | 1.391 (8) | . | . | no |
| C15 | C16 | 1.395 (7) | . | . | no |
| C16 | C110 | 1.518 (6) | . | . | no |
| C17 | C18 | 1.534 (6) | . | . | no |
| C17 | C19 | 1.526 (6) | . | . | no |
| C110 | C111 | 1.534 (7) | . | . | no |
| C110 | C112 | 1.526 (6) | . | . | no |
| C13 | H13 | 0.9500 | . | . | no |
| C113 | C114 | 1.565 (6) | . | . | no |
| C14 | H14 | 0.9500 | . | . | no |
| C114 | C116 | 1.539 (7) | . | . | no |
| C114 | C117 | 1.540 (5) | . | . | no |
| C114 | C115 | 1.529 (7) | . | . | no |
| C15 | H15 | 0.9500 | . | . | no |
| C17 | H17 | 1.0000 | . | . | no |
| C18 | H18" | 0.9800 | . | . | no |
| C18 | H18 | 0.9800 | . | . | no |
| C18 | H18' | 0.9800 | . | . | no |
| C118 | C119 | 1.420 (7) | . | . | no |
| C118 | C123 | 1.398 (7) | . | . | no |
| C19 | H19' | 0.9800 | . | . | no |
| C119 | C120 | 1.386 (8) | . | . | no |
| C19 | H19 | 0.9800 | . | . | no |
| C119 | C124 | 1.503 (7) | . | . | no |
| C19 | H19" | 0.9800 | . | . | no |
| C120 | C121 | 1.378 (7) | . | . | no |
| C121 | C122 | 1.363 (7) | . | . | no |
| C122 | C123 | 1.418 (7) | . | . | no |
| C123 | C127 | 1.503 (7) | . | . | no |
| C124 | C126 | 1.523 (6) | . | . | no |
| C124 | C125 | 1.536 (7) | . | . | no |
| C127 | C129 | 1.541 (6) | . | . | no |
| C127 | C128 | 1.533 (8) | . | . | no |
| C130 | C131 | 1.475 (7) | . | . | no |
| C131 | C132 | 1.384 (7) | . | . | no |
| C131 | C136 | 1.402 (6) | . | . | no |
| C132 | C133 | 1.386 (8) | . | . | no |
| C133 | C134 | 1.374 (9) | . | . | no |
| C134 | C135 | 1.403 (8) | . | . | no |
| C135 | C136 | 1.382 (7) | . | . | no |
| C137 | C138 | 1.500 (8) | . | . | no |
| C138 | C139 | 1.483 (9) | . | . | no |
| C139 | C140 | 1.515 (8) | . | . | no |
| C141 | C142 | 1.506 (7) | . | . | no |
| C142 | C143 | 1.519 (8) | . | . | no |
| C143 | C144 | 1.466 (9) | . | . | no |
| C145 | C146 | 1.485 (8) | . | . | no |
| C146 | C147 | 1.490 (9) | . | . | no |
| C147 | C148 | 1.509 (8) | . | . | no |
| C110 | H110 | 1.0000 | . | . | no |
| C111 | H111" | 0.9800 | . | . | no |

| | | | | | |
|------|-------|-----------|---|---|-----|
| C111 | H111' | 0.9800 | . | . | no |
| C111 | H111 | 0.9800 | . | . | no |
| C112 | H112 | 0.9800 | . | . | no |
| C112 | H112" | 0.9800 | . | . | no |
| C112 | H112' | 0.9800 | . | . | no |
| C115 | H115' | 0.9800 | . | . | no |
| C115 | H115" | 0.9800 | . | . | no |
| C115 | H115 | 0.9800 | . | . | no |
| C116 | H116' | 0.9800 | . | . | no |
| C116 | H116 | 0.9800 | . | . | no |
| C116 | H116" | 0.9800 | . | . | no |
| C117 | H117" | 0.9800 | . | . | no |
| C117 | H117' | 0.9800 | . | . | no |
| C117 | H117 | 0.9800 | . | . | no |
| C120 | H120 | 0.9500 | . | . | no |
| C121 | H121 | 0.9500 | . | . | no |
| C21 | B2 | 1.656 (7) | . | . | yes |
| C21 | C26 | 1.398 (7) | . | . | no |
| C21 | C22 | 1.407 (7) | . | . | no |
| C122 | H122 | 0.9500 | . | . | no |
| C22 | C23 | 1.376 (7) | . | . | no |
| C23 | C24 | 1.386 (8) | . | . | no |
| C24 | C25 | 1.386 (7) | . | . | no |
| C124 | H124 | 1.0000 | . | . | no |
| C25 | C26 | 1.394 (7) | . | . | no |
| C125 | H125 | 0.9800 | . | . | no |
| C125 | H125" | 0.9800 | . | . | no |
| C125 | H125' | 0.9800 | . | . | no |
| C126 | H126 | 0.9800 | . | . | no |
| C126 | H126' | 0.9800 | . | . | no |
| C126 | H126" | 0.9800 | . | . | no |
| C27 | B2 | 1.646 (6) | . | . | yes |
| C127 | H127 | 1.0000 | . | . | no |
| C27 | C28 | 1.412 (8) | . | . | no |
| C27 | C212 | 1.390 (6) | . | . | no |
| C128 | H128" | 0.9800 | . | . | no |
| C128 | H128 | 0.9800 | . | . | no |
| C128 | H128' | 0.9800 | . | . | no |
| C28 | C29 | 1.391 (9) | . | . | no |
| C129 | H129 | 0.9800 | . | . | no |
| C29 | C210 | 1.373 (9) | . | . | no |
| C129 | H129' | 0.9800 | . | . | no |
| C129 | H129" | 0.9800 | . | . | no |
| C130 | H130' | 0.9900 | . | . | no |
| C130 | H130 | 0.9900 | . | . | no |
| C132 | H132 | 0.9500 | . | . | no |
| C133 | H133 | 0.9500 | . | . | no |
| C134 | H134 | 0.9500 | . | . | no |
| C135 | H135 | 0.9500 | . | . | no |
| C136 | H136 | 0.9500 | . | . | no |
| C137 | H137 | 0.9900 | . | . | no |
| C137 | H137' | 0.9900 | . | . | no |
| C138 | H138 | 0.9900 | . | . | no |
| C138 | H138' | 0.9900 | . | . | no |
| C139 | H139 | 0.9900 | . | . | no |
| C139 | H139' | 0.9900 | . | . | no |
| C140 | H140 | 0.9900 | . | . | no |
| C140 | H140' | 0.9900 | . | . | no |
| C141 | H141 | 0.9900 | . | . | no |
| C141 | H141' | 0.9900 | . | . | no |
| C142 | H142' | 0.9900 | . | . | no |

| | | | | | |
|------|-------|------------|---|---|-----|
| C142 | H142 | 0.9900 | . | . | no |
| C143 | H143 | 0.9900 | . | . | no |
| C143 | H143' | 0.9900 | . | . | no |
| C144 | H144 | 0.9900 | . | . | no |
| C144 | H144' | 0.9900 | . | . | no |
| C145 | H145' | 0.9900 | . | . | no |
| C145 | H145 | 0.9900 | . | . | no |
| C146 | H146' | 0.9900 | . | . | no |
| C146 | H146 | 0.9900 | . | . | no |
| C147 | H147 | 0.9900 | . | . | no |
| C147 | H147' | 0.9900 | . | . | no |
| C148 | H148 | 0.9900 | . | . | no |
| C148 | H148' | 0.9900 | . | . | no |
| C22 | H22 | 0.9500 | . | . | no |
| C23 | H23 | 0.9500 | . | . | no |
| C24 | H24 | 0.9500 | . | . | no |
| C25 | H25 | 0.9500 | . | . | no |
| C26 | H26 | 0.9500 | . | . | no |
| C28 | H28 | 0.9500 | . | . | no |
| C29 | H29 | 0.9500 | . | . | no |
| C210 | C211 | 1.371 (10) | . | . | no |
| C211 | C212 | 1.388 (8) | . | . | no |
| C213 | C218 | 1.406 (7) | . | . | no |
| C213 | B2 | 1.644 (7) | . | . | yes |
| C213 | C214 | 1.417 (6) | . | . | no |
| C214 | C215 | 1.392 (7) | . | . | no |
| C215 | C216 | 1.379 (7) | . | . | no |
| C216 | C217 | 1.381 (8) | . | . | no |
| C217 | C218 | 1.393 (7) | . | . | no |
| C219 | C224 | 1.404 (7) | . | . | no |
| C219 | B2 | 1.651 (6) | . | . | yes |
| C219 | C220 | 1.403 (6) | . | . | no |
| C220 | C221 | 1.389 (8) | . | . | no |
| C221 | C222 | 1.380 (8) | . | . | no |
| C222 | C223 | 1.374 (9) | . | . | no |
| C223 | C224 | 1.398 (8) | . | . | no |
| C31 | C32 | 1.442 (17) | . | . | no |
| C32 | C33 | 1.32 (2) | . | . | no |
| C33 | C34 | 1.414 (19) | . | . | no |
| C210 | H210 | 0.9500 | . | . | no |
| C211 | H211 | 0.9500 | . | . | no |
| C212 | H212 | 0.9500 | . | . | no |
| C214 | H214 | 0.9500 | . | . | no |
| C215 | H215 | 0.9500 | . | . | no |
| C216 | H216 | 0.9500 | . | . | no |
| C217 | H217 | 0.9500 | . | . | no |
| C218 | H218 | 0.9500 | . | . | no |
| C220 | H220 | 0.9500 | . | . | no |
| C221 | H221 | 0.9500 | . | . | no |
| C222 | H222 | 0.9500 | . | . | no |
| C223 | H223 | 0.9500 | . | . | no |
| C224 | H224 | 0.9500 | . | . | no |
| C31 | H31 | 0.9900 | . | . | no |
| C31 | H31' | 0.9900 | . | . | no |
| C32 | H32 | 0.9900 | . | . | no |
| C32 | H32' | 0.9900 | . | . | no |
| C33 | H33 | 0.9900 | . | . | no |
| C33 | H33' | 0.9900 | . | . | no |
| C34 | H34 | 0.9900 | . | . | no |
| C34 | H34' | 0.9900 | . | . | no |

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loop_
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
O11      La1      O12      73.02(10)      .      .      .      yes
O11      La1      O13      135.22(10)     .      .      .      yes
O11      La1      N11      88.13(10)     .      .      .      yes
O11      La1      N12      139.99(10)     .      .      .      yes
O11      La1      C130     89.08(14)     .      .      .      yes
O12      La1      O13      71.95(10)     .      .      .      yes
O12      La1      N11      126.67(11)     .      .      .      yes
O12      La1      N12      126.35(10)     .      .      .      yes
O12      La1      C130     116.96(12)     .      .      .      yes
O13      La1      N11      135.63(10)     .      .      .      yes
O13      La1      N12      84.09(10)     .      .      .      yes
O13      La1      C130     82.78(14)     .      .      .      yes
N11      La1      N12      51.91(11)     .      .      .      yes
N11      La1      C130     111.93(13)     .      .      .      yes
N12      La1      C130     106.20(13)     .      .      .      yes
La1      O11      C137     122.2(3)      .      .      .      yes
La1      O11      C140     127.8(3)      .      .      .      yes
C137     O11      C140     109.7(4)      .      .      .      yes
La1      O12      C141     123.0(2)      .      .      .      yes
La1      O12      C144     131.7(3)      .      .      .      yes
C141     O12      C144     105.3(4)      .      .      .      yes
La1      O13      C145     135.3(3)      .      .      .      yes
La1      O13      C148     115.4(3)      .      .      .      yes
C145     O13      C148     108.7(3)      .      .      .      yes
C31      O31      C34      110.8(8)      .      .      .      yes
La1      N11      C113     99.7(2)       .      .      .      yes
C11      N11      C113     129.2(3)      .      .      .      yes
La1      N11      C11      129.0(2)      .      .      .      yes
La1      N12      C113     96.6(2)       .      .      .      yes
C113     N12      C118     130.0(3)      .      .      .      yes
La1      N12      C118     133.4(2)      .      .      .      yes
N11      C11      C12      120.9(4)      .      .      .      yes
C12      C11      C16      120.4(4)      .      .      .      no
N11      C11      C16      117.8(4)      .      .      .      yes
C11      C12      C13      118.1(5)      .      .      .      no
C11      C12      C17      122.5(4)      .      .      .      no
C13      C12      C17      119.3(4)      .      .      .      no
C12      C13      C14      122.4(4)      .      .      .      no
C13      C14      C15      119.3(5)      .      .      .      no
C14      C15      C16      121.3(5)      .      .      .      no
C11      C16      C110     121.8(3)      .      .      .      no
C15      C16      C110     119.6(4)      .      .      .      no
C11      C16      C15      118.5(4)      .      .      .      no
C12      C17      C18      110.3(4)      .      .      .      no
C18      C17      C19      109.2(4)      .      .      .      no
C12      C17      C19      113.1(4)      .      .      .      no
C16      C110     C111     114.0(4)      .      .      .      no
C111     C110     C112     109.4(4)      .      .      .      no
C16      C110     C112     111.2(4)      .      .      .      no
N11      C113     N12      111.7(3)      .      .      .      yes
N11      C113     C114     122.3(3)      .      .      .      yes
C14      C13      H13      119.00        .      .      .      no

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| | | | | | | | |
|------|------|------|----------|---|---|---|-----|
| C12 | C13 | H13 | 119.00 | . | . | . | no |
| N12 | C113 | C114 | 125.7(3) | . | . | . | yes |
| C115 | C114 | C116 | 108.7(4) | . | . | . | no |
| C113 | C114 | C116 | 112.5(3) | . | . | . | no |
| C116 | C114 | C117 | 106.6(4) | . | . | . | no |
| C13 | C14 | H14 | 120.00 | . | . | . | no |
| C115 | C114 | C117 | 106.6(4) | . | . | . | no |
| C113 | C114 | C115 | 107.2(3) | . | . | . | no |
| C15 | C14 | H14 | 120.00 | . | . | . | no |
| C113 | C114 | C117 | 115.0(3) | . | . | . | no |
| C16 | C15 | H15 | 119.00 | . | . | . | no |
| C14 | C15 | H15 | 119.00 | . | . | . | no |
| C18 | C17 | H17 | 108.00 | . | . | . | no |
| C19 | C17 | H17 | 108.00 | . | . | . | no |
| C12 | C17 | H17 | 108.00 | . | . | . | no |
| C119 | C118 | C123 | 120.0(4) | . | . | . | no |
| C17 | C18 | H18" | 109.00 | . | . | . | no |
| H18 | C18 | H18' | 110.00 | . | . | . | no |
| C17 | C18 | H18' | 110.00 | . | . | . | no |
| H18' | C18 | H18" | 109.00 | . | . | . | no |
| N12 | C118 | C119 | 119.4(4) | . | . | . | yes |
| N12 | C118 | C123 | 120.1(4) | . | . | . | yes |
| C17 | C18 | H18 | 109.00 | . | . | . | no |
| H18 | C18 | H18" | 109.00 | . | . | . | no |
| C118 | C119 | C120 | 119.1(5) | . | . | . | no |
| C118 | C119 | C124 | 121.8(5) | . | . | . | no |
| H19' | C19 | H19" | 109.00 | . | . | . | no |
| H19 | C19 | H19" | 109.00 | . | . | . | no |
| C17 | C19 | H19 | 109.00 | . | . | . | no |
| C17 | C19 | H19' | 110.00 | . | . | . | no |
| C17 | C19 | H19" | 110.00 | . | . | . | no |
| H19 | C19 | H19' | 109.00 | . | . | . | no |
| C120 | C119 | C124 | 119.2(5) | . | . | . | no |
| C119 | C120 | C121 | 121.2(5) | . | . | . | no |
| C120 | C121 | C122 | 120.0(5) | . | . | . | no |
| C121 | C122 | C123 | 121.5(5) | . | . | . | no |
| C118 | C123 | C122 | 118.2(4) | . | . | . | no |
| C118 | C123 | C127 | 122.2(4) | . | . | . | no |
| C122 | C123 | C127 | 119.7(4) | . | . | . | no |
| C125 | C124 | C126 | 110.5(4) | . | . | . | no |
| C119 | C124 | C125 | 114.6(4) | . | . | . | no |
| C119 | C124 | C126 | 110.7(4) | . | . | . | no |
| C123 | C127 | C128 | 112.5(4) | . | . | . | no |
| C123 | C127 | C129 | 111.5(4) | . | . | . | no |
| C128 | C127 | C129 | 109.3(4) | . | . | . | no |
| La1 | C130 | C131 | 132.0(3) | . | . | . | yes |
| C132 | C131 | C136 | 116.6(5) | . | . | . | no |
| C130 | C131 | C132 | 121.0(4) | . | . | . | no |
| C130 | C131 | C136 | 122.4(4) | . | . | . | no |
| C131 | C132 | C133 | 122.0(6) | . | . | . | no |
| C132 | C133 | C134 | 121.0(5) | . | . | . | no |
| C133 | C134 | C135 | 118.2(5) | . | . | . | no |
| C134 | C135 | C136 | 120.3(5) | . | . | . | no |
| C131 | C136 | C135 | 121.8(5) | . | . | . | no |
| O11 | C137 | C138 | 104.1(4) | . | . | . | yes |
| C137 | C138 | C139 | 104.4(5) | . | . | . | no |
| C138 | C139 | C140 | 101.9(5) | . | . | . | no |
| O11 | C140 | C139 | 105.1(4) | . | . | . | yes |
| O12 | C141 | C142 | 104.2(4) | . | . | . | yes |
| C141 | C142 | C143 | 102.5(4) | . | . | . | no |
| C142 | C143 | C144 | 104.8(5) | . | . | . | no |

| | | | | | | | |
|-------|------|-------|-----------|---|---|---|-----|
| O12 | C144 | C143 | 109.5 (5) | . | . | . | yes |
| O13 | C145 | C146 | 104.7 (4) | . | . | . | yes |
| C145 | C146 | C147 | 103.6 (4) | . | . | . | no |
| C146 | C147 | C148 | 104.7 (5) | . | . | . | no |
| O13 | C148 | C147 | 105.5 (4) | . | . | . | yes |
| C16 | C110 | H110 | 107.00 | . | . | . | no |
| C112 | C110 | H110 | 107.00 | . | . | . | no |
| C111 | C110 | H110 | 107.00 | . | . | . | no |
| C110 | C111 | H111" | 109.00 | . | . | . | no |
| C110 | C111 | H111 | 109.00 | . | . | . | no |
| H111' | C111 | H111" | 109.00 | . | . | . | no |
| H111' | C111 | H111 | 109.00 | . | . | . | no |
| H111" | C111 | H111 | 110.00 | . | . | . | no |
| C110 | C111 | H111' | 109.00 | . | . | . | no |
| C110 | C112 | H112' | 109.00 | . | . | . | no |
| C110 | C112 | H112 | 109.00 | . | . | . | no |
| H112' | C112 | H112" | 109.00 | . | . | . | no |
| H112' | C112 | H112 | 109.00 | . | . | . | no |
| H112" | C112 | H112 | 109.00 | . | . | . | no |
| C110 | C112 | H112" | 110.00 | . | . | . | no |
| C114 | C115 | H115' | 110.00 | . | . | . | no |
| C114 | C115 | H115" | 109.00 | . | . | . | no |
| H115' | C115 | H115" | 109.00 | . | . | . | no |
| H115' | C115 | H115 | 109.00 | . | . | . | no |
| H115" | C115 | H115 | 109.00 | . | . | . | no |
| C114 | C115 | H115 | 110.00 | . | . | . | no |
| C114 | C116 | H116' | 109.00 | . | . | . | no |
| C114 | C116 | H116 | 109.00 | . | . | . | no |
| H116' | C116 | H116" | 109.00 | . | . | . | no |
| C114 | C116 | H116" | 109.00 | . | . | . | no |
| H116" | C116 | H116 | 109.00 | . | . | . | no |
| H116' | C116 | H116 | 109.00 | . | . | . | no |
| C114 | C117 | H117' | 109.00 | . | . | . | no |
| C114 | C117 | H117" | 109.00 | . | . | . | no |
| H117' | C117 | H117" | 109.00 | . | . | . | no |
| H117' | C117 | H117 | 110.00 | . | . | . | no |
| C114 | C117 | H117 | 109.00 | . | . | . | no |
| H117" | C117 | H117 | 110.00 | . | . | . | no |
| C121 | C120 | H120 | 119.00 | . | . | . | no |
| C119 | C120 | H120 | 119.00 | . | . | . | no |
| C122 | C121 | H121 | 120.00 | . | . | . | no |
| C26 | C21 | B2 | 126.7 (4) | . | . | . | yes |
| C22 | C21 | B2 | 118.5 (4) | . | . | . | yes |
| C120 | C121 | H121 | 120.00 | . | . | . | no |
| C22 | C21 | C26 | 114.8 (4) | . | . | . | no |
| C123 | C122 | H122 | 119.00 | . | . | . | no |
| C21 | C22 | C23 | 123.5 (5) | . | . | . | no |
| C121 | C122 | H122 | 119.00 | . | . | . | no |
| C22 | C23 | C24 | 120.0 (5) | . | . | . | no |
| C126 | C124 | H124 | 107.00 | . | . | . | no |
| C125 | C124 | H124 | 107.00 | . | . | . | no |
| C119 | C124 | H124 | 107.00 | . | . | . | no |
| C23 | C24 | C25 | 118.8 (5) | . | . | . | no |
| C124 | C125 | H125' | 109.00 | . | . | . | no |
| C124 | C125 | H125" | 110.00 | . | . | . | no |
| C124 | C125 | H125 | 109.00 | . | . | . | no |
| H125' | C125 | H125" | 109.00 | . | . | . | no |
| H125' | C125 | H125 | 109.00 | . | . | . | no |
| H125" | C125 | H125 | 110.00 | . | . | . | no |
| C24 | C25 | C26 | 120.3 (5) | . | . | . | no |
| C124 | C126 | H126' | 110.00 | . | . | . | no |

| | | | | | | | |
|-------|------|-------|-----------|---|---|---|-----|
| C21 | C26 | C25 | 122.7 (5) | . | . | . | no |
| H126' | C126 | H126 | 110.00 | . | . | . | no |
| C124 | C126 | H126 | 110.00 | . | . | . | no |
| H126' | C126 | H126" | 109.00 | . | . | . | no |
| C124 | C126 | H126" | 109.00 | . | . | . | no |
| H126" | C126 | H126 | 109.00 | . | . | . | no |
| C123 | C127 | H127 | 108.00 | . | . | . | no |
| C28 | C27 | C212 | 115.1 (5) | . | . | . | no |
| C129 | C127 | H127 | 108.00 | . | . | . | no |
| C28 | C27 | B2 | 121.1 (4) | . | . | . | yes |
| C212 | C27 | B2 | 123.7 (5) | . | . | . | yes |
| C128 | C127 | H127 | 108.00 | . | . | . | no |
| H128" | C128 | H128 | 109.00 | . | . | . | no |
| C27 | C28 | C29 | 122.1 (5) | . | . | . | no |
| H128' | C128 | H128 | 109.00 | . | . | . | no |
| C127 | C128 | H128 | 109.00 | . | . | . | no |
| C127 | C128 | H128' | 109.00 | . | . | . | no |
| C127 | C128 | H128" | 109.00 | . | . | . | no |
| H128' | C128 | H128" | 110.00 | . | . | . | no |
| C127 | C129 | H129 | 110.00 | . | . | . | no |
| C127 | C129 | H129' | 109.00 | . | . | . | no |
| C28 | C29 | C210 | 120.0 (6) | . | . | . | no |
| H129' | C129 | H129 | 110.00 | . | . | . | no |
| C127 | C129 | H129" | 109.00 | . | . | . | no |
| H129' | C129 | H129" | 109.00 | . | . | . | no |
| H129" | C129 | H129 | 110.00 | . | . | . | no |
| C131 | C130 | H130' | 104.00 | . | . | . | no |
| La1 | C130 | H130' | 104.00 | . | . | . | no |
| C131 | C130 | H130 | 104.00 | . | . | . | no |
| H130' | C130 | H130 | 106.00 | . | . | . | no |
| C131 | C132 | H132 | 119.00 | . | . | . | no |
| C133 | C132 | H132 | 119.00 | . | . | . | no |
| C134 | C133 | H133 | 119.00 | . | . | . | no |
| C132 | C133 | H133 | 120.00 | . | . | . | no |
| C135 | C134 | H134 | 121.00 | . | . | . | no |
| C133 | C134 | H134 | 121.00 | . | . | . | no |
| C134 | C135 | H135 | 120.00 | . | . | . | no |
| C136 | C135 | H135 | 120.00 | . | . | . | no |
| C135 | C136 | H136 | 119.00 | . | . | . | no |
| C131 | C136 | H136 | 119.00 | . | . | . | no |
| O11 | C137 | H137' | 111.00 | . | . | . | no |
| C138 | C137 | H137' | 111.00 | . | . | . | no |
| C138 | C137 | H137 | 111.00 | . | . | . | no |
| O11 | C137 | H137 | 111.00 | . | . | . | no |
| H137' | C137 | H137 | 109.00 | . | . | . | no |
| H138' | C138 | H138 | 109.00 | . | . | . | no |
| C137 | C138 | H138' | 111.00 | . | . | . | no |
| C137 | C138 | H138 | 111.00 | . | . | . | no |
| C139 | C138 | H138 | 111.00 | . | . | . | no |
| C139 | C138 | H138' | 111.00 | . | . | . | no |
| C140 | C139 | H139 | 111.00 | . | . | . | no |
| C140 | C139 | H139' | 111.00 | . | . | . | no |
| C138 | C139 | H139' | 111.00 | . | . | . | no |
| C138 | C139 | H139 | 111.00 | . | . | . | no |
| H139' | C139 | H139 | 109.00 | . | . | . | no |
| O11 | C140 | H140 | 111.00 | . | . | . | no |
| H140' | C140 | H140 | 109.00 | . | . | . | no |
| O11 | C140 | H140' | 111.00 | . | . | . | no |
| C139 | C140 | H140' | 111.00 | . | . | . | no |
| C139 | C140 | H140 | 111.00 | . | . | . | no |

| | | | | | | | |
|-------|------|-------|----------|---|---|---|-----|
| O12 | C141 | H141' | 111.00 | . | . | . | no |
| C142 | C141 | H141 | 111.00 | . | . | . | no |
| O12 | C141 | H141 | 111.00 | . | . | . | no |
| C142 | C141 | H141' | 111.00 | . | . | . | no |
| H141' | C141 | H141 | 109.00 | . | . | . | no |
| C143 | C142 | H142' | 111.00 | . | . | . | no |
| C141 | C142 | H142' | 111.00 | . | . | . | no |
| C143 | C142 | H142 | 111.00 | . | . | . | no |
| H142' | C142 | H142 | 109.00 | . | . | . | no |
| C141 | C142 | H142 | 111.00 | . | . | . | no |
| H143' | C143 | H143 | 109.00 | . | . | . | no |
| C144 | C143 | H143 | 111.00 | . | . | . | no |
| C142 | C143 | H143' | 111.00 | . | . | . | no |
| C142 | C143 | H143 | 111.00 | . | . | . | no |
| C144 | C143 | H143' | 111.00 | . | . | . | no |
| O12 | C144 | H144 | 110.00 | . | . | . | no |
| C143 | C144 | H144' | 110.00 | . | . | . | no |
| O12 | C144 | H144' | 110.00 | . | . | . | no |
| H144' | C144 | H144 | 108.00 | . | . | . | no |
| C143 | C144 | H144 | 110.00 | . | . | . | no |
| C146 | C145 | H145 | 111.00 | . | . | . | no |
| C146 | C145 | H145' | 111.00 | . | . | . | no |
| O13 | C145 | H145' | 111.00 | . | . | . | no |
| O13 | C145 | H145 | 111.00 | . | . | . | no |
| H145' | C145 | H145 | 109.00 | . | . | . | no |
| C145 | C146 | H146 | 111.00 | . | . | . | no |
| C147 | C146 | H146' | 111.00 | . | . | . | no |
| H146' | C146 | H146 | 109.00 | . | . | . | no |
| C145 | C146 | H146' | 111.00 | . | . | . | no |
| C147 | C146 | H146 | 111.00 | . | . | . | no |
| C146 | C147 | H147' | 111.00 | . | . | . | no |
| C146 | C147 | H147 | 111.00 | . | . | . | no |
| H147' | C147 | H147 | 109.00 | . | . | . | no |
| C148 | C147 | H147' | 111.00 | . | . | . | no |
| C148 | C147 | H147 | 111.00 | . | . | . | no |
| C147 | C148 | H148 | 111.00 | . | . | . | no |
| O13 | C148 | H148' | 111.00 | . | . | . | no |
| O13 | C148 | H148 | 111.00 | . | . | . | no |
| H148' | C148 | H148 | 109.00 | . | . | . | no |
| C147 | C148 | H148' | 111.00 | . | . | . | no |
| C21 | C22 | H22 | 118.00 | . | . | . | no |
| C23 | C22 | H22 | 118.00 | . | . | . | no |
| C24 | C23 | H23 | 120.00 | . | . | . | no |
| C22 | C23 | H23 | 120.00 | . | . | . | no |
| C23 | C24 | H24 | 121.00 | . | . | . | no |
| C25 | C24 | H24 | 121.00 | . | . | . | no |
| C26 | C25 | H25 | 120.00 | . | . | . | no |
| C24 | C25 | H25 | 120.00 | . | . | . | no |
| C25 | C26 | H26 | 119.00 | . | . | . | no |
| C21 | C26 | H26 | 119.00 | . | . | . | no |
| C29 | C28 | H28 | 119.00 | . | . | . | no |
| C27 | C28 | H28 | 119.00 | . | . | . | no |
| C28 | C29 | H29 | 120.00 | . | . | . | no |
| C210 | C29 | H29 | 120.00 | . | . | . | no |
| C29 | C210 | C211 | 119.9(6) | . | . | . | no |
| C210 | C211 | C212 | 119.6(6) | . | . | . | no |
| C27 | C212 | C211 | 123.2(5) | . | . | . | no |
| C218 | C213 | B2 | 123.3(4) | . | . | . | yes |
| C214 | C213 | C218 | 113.8(4) | . | . | . | no |
| C214 | C213 | B2 | 122.8(4) | . | . | . | yes |
| C213 | C214 | C215 | 123.3(4) | . | . | . | no |

| | | | | | | | |
|------|------|------|-----------|---|---|---|-----|
| C214 | C215 | C216 | 119.9(4) | . | . | . | no |
| C215 | C216 | C217 | 119.6(5) | . | . | . | no |
| C216 | C217 | C218 | 119.7(5) | . | . | . | no |
| C213 | C218 | C217 | 123.6(4) | . | . | . | no |
| C220 | C219 | B2 | 124.4(4) | . | . | . | yes |
| C220 | C219 | C224 | 114.3(4) | . | . | . | no |
| C224 | C219 | B2 | 121.2(4) | . | . | . | yes |
| C219 | C220 | C221 | 123.0(5) | . | . | . | no |
| C220 | C221 | C222 | 120.9(6) | . | . | . | no |
| C221 | C222 | C223 | 118.2(5) | . | . | . | no |
| C222 | C223 | C224 | 120.7(5) | . | . | . | no |
| C219 | C224 | C223 | 122.8(5) | . | . | . | no |
| O31 | C31 | C32 | 103.8(10) | . | . | . | yes |
| C31 | C32 | C33 | 110.1(13) | . | . | . | no |
| C32 | C33 | C34 | 108.4(11) | . | . | . | no |
| O31 | C34 | C33 | 104.7(9) | . | . | . | yes |
| C211 | C210 | H210 | 120.00 | . | . | . | no |
| C29 | C210 | H210 | 120.00 | . | . | . | no |
| C210 | C211 | H211 | 120.00 | . | . | . | no |
| C212 | C211 | H211 | 120.00 | . | . | . | no |
| C211 | C212 | H212 | 118.00 | . | . | . | no |
| C27 | C212 | H212 | 118.00 | . | . | . | no |
| C213 | C214 | H214 | 118.00 | . | . | . | no |
| C215 | C214 | H214 | 118.00 | . | . | . | no |
| C216 | C215 | H215 | 120.00 | . | . | . | no |
| C214 | C215 | H215 | 120.00 | . | . | . | no |
| C217 | C216 | H216 | 120.00 | . | . | . | no |
| C215 | C216 | H216 | 120.00 | . | . | . | no |
| C216 | C217 | H217 | 120.00 | . | . | . | no |
| C218 | C217 | H217 | 120.00 | . | . | . | no |
| C213 | C218 | H218 | 118.00 | . | . | . | no |
| C217 | C218 | H218 | 118.00 | . | . | . | no |
| C219 | C220 | H220 | 118.00 | . | . | . | no |
| C221 | C220 | H220 | 119.00 | . | . | . | no |
| C222 | C221 | H221 | 120.00 | . | . | . | no |
| C220 | C221 | H221 | 120.00 | . | . | . | no |
| C221 | C222 | H222 | 121.00 | . | . | . | no |
| C223 | C222 | H222 | 121.00 | . | . | . | no |
| C224 | C223 | H223 | 120.00 | . | . | . | no |
| C222 | C223 | H223 | 120.00 | . | . | . | no |
| C219 | C224 | H224 | 119.00 | . | . | . | no |
| C223 | C224 | H224 | 119.00 | . | . | . | no |
| O31 | C31 | H31 | 111.00 | . | . | . | no |
| C32 | C31 | H31 | 111.00 | . | . | . | no |
| C32 | C31 | H31' | 111.00 | . | . | . | no |
| H31 | C31 | H31' | 109.00 | . | . | . | no |
| O31 | C31 | H31' | 111.00 | . | . | . | no |
| C31 | C32 | H32' | 110.00 | . | . | . | no |
| C33 | C32 | H32 | 110.00 | . | . | . | no |
| C31 | C32 | H32 | 110.00 | . | . | . | no |
| H32 | C32 | H32' | 108.00 | . | . | . | no |
| C33 | C32 | H32' | 110.00 | . | . | . | no |
| C34 | C33 | H33' | 110.00 | . | . | . | no |
| H33 | C33 | H33' | 108.00 | . | . | . | no |
| C34 | C33 | H33 | 110.00 | . | . | . | no |
| C32 | C33 | H33 | 110.00 | . | . | . | no |
| C32 | C33 | H33' | 110.00 | . | . | . | no |
| O31 | C34 | H34' | 111.00 | . | . | . | no |
| C33 | C34 | H34 | 111.00 | . | . | . | no |
| O31 | C34 | H34 | 111.00 | . | . | . | no |
| H34 | C34 | H34' | 109.00 | . | . | . | no |

| | | | | | | | |
|------|-----|------|----------|---|---|---|-----|
| C33 | C34 | H34' | 111.00 | . | . | . | no |
| C21 | B2 | C213 | 113.4(4) | . | . | . | yes |
| C21 | B2 | C219 | 107.0(4) | . | . | . | yes |
| C27 | B2 | C219 | 110.6(4) | . | . | . | yes |
| C213 | B2 | C219 | 108.7(3) | . | . | . | yes |
| C27 | B2 | C213 | 108.3(4) | . | . | . | yes |
| C21 | B2 | C27 | 108.9(3) | . | . | . | yes |

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

| | | | | | | | | |
|------|-----|-----|------|-----------|---|---|---|----|
| O12 | La1 | O11 | C137 | -92.1(3) | . | . | . | no |
| O12 | La1 | O11 | C140 | 80.7(4) | . | . | . | no |
| O13 | La1 | O11 | C137 | -52.2(3) | . | . | . | no |
| O13 | La1 | O11 | C140 | 120.5(4) | . | . | . | no |
| N11 | La1 | O11 | C137 | 138.5(3) | . | . | . | no |
| N11 | La1 | O11 | C140 | -48.7(4) | . | . | . | no |
| N12 | La1 | O11 | C137 | 141.1(3) | . | . | . | no |
| N12 | La1 | O11 | C140 | -46.2(4) | . | . | . | no |
| C130 | La1 | O11 | C137 | 26.6(3) | . | . | . | no |
| C130 | La1 | O11 | C140 | -160.7(4) | . | . | . | no |
| O11 | La1 | O12 | C141 | -155.2(3) | . | . | . | no |
| O11 | La1 | O12 | C144 | 28.4(4) | . | . | . | no |
| O13 | La1 | O12 | C141 | 53.1(3) | . | . | . | no |
| O13 | La1 | O12 | C144 | -123.3(5) | . | . | . | no |
| N11 | La1 | O12 | C141 | -80.9(3) | . | . | . | no |
| N11 | La1 | O12 | C144 | 102.7(5) | . | . | . | no |
| N12 | La1 | O12 | C141 | -14.9(4) | . | . | . | no |
| N12 | La1 | O12 | C144 | 168.7(4) | . | . | . | no |
| C130 | La1 | O12 | C141 | 124.8(3) | . | . | . | no |
| C130 | La1 | O12 | C144 | -51.6(5) | . | . | . | no |
| O11 | La1 | O13 | C145 | -137.7(3) | . | . | . | no |
| O11 | La1 | O13 | C148 | 32.7(3) | . | . | . | no |
| O12 | La1 | O13 | C145 | -97.6(4) | . | . | . | no |
| O12 | La1 | O13 | C148 | 72.8(3) | . | . | . | no |
| N11 | La1 | O13 | C145 | 26.8(4) | . | . | . | no |
| N11 | La1 | O13 | C148 | -162.8(3) | . | . | . | no |
| N12 | La1 | O13 | C145 | 33.8(4) | . | . | . | no |
| N12 | La1 | O13 | C148 | -155.8(3) | . | . | . | no |
| C130 | La1 | O13 | C145 | 141.0(4) | . | . | . | no |
| C130 | La1 | O13 | C148 | -48.6(3) | . | . | . | no |
| O11 | La1 | N11 | C11 | 15.5(4) | . | . | . | no |
| O11 | La1 | N11 | C113 | 180.0(2) | . | . | . | no |
| O12 | La1 | N11 | C11 | -51.6(4) | . | . | . | no |
| O12 | La1 | N11 | C113 | 112.8(2) | . | . | . | no |
| O13 | La1 | N11 | C11 | -153.7(3) | . | . | . | no |
| O13 | La1 | N11 | C113 | 10.8(3) | . | . | . | no |
| N12 | La1 | N11 | C11 | -162.5(4) | . | . | . | no |
| N12 | La1 | N11 | C113 | 2.0(2) | . | . | . | no |
| C130 | La1 | N11 | C11 | 103.7(4) | . | . | . | no |
| C130 | La1 | N11 | C113 | -91.8(3) | . | . | . | no |
| O11 | La1 | N12 | C113 | -5.2(3) | . | . | . | no |
| O11 | La1 | N12 | C118 | 175.3(3) | . | . | . | no |

| | | | | | | | | | |
|------|-----|------|------|------------|---|---|---|---|----|
| O12 | La1 | N12 | C113 | -113.4 (2) | . | . | . | . | no |
| O12 | La1 | N12 | C118 | 67.0 (4) | . | . | . | . | no |
| O13 | La1 | N12 | C113 | -175.9 (2) | . | . | . | . | no |
| O13 | La1 | N12 | C118 | 4.6 (4) | . | . | . | . | no |
| N11 | La1 | N12 | C113 | -2.0 (2) | . | . | . | . | no |
| N11 | La1 | N12 | C118 | 178.5 (4) | . | . | . | . | no |
| C130 | La1 | N12 | C113 | 103.4 (3) | . | . | . | . | no |
| C130 | La1 | N12 | C118 | -76.1 (4) | . | . | . | . | no |
| O11 | La1 | C130 | C131 | 65.7 (4) | . | . | . | . | no |
| O12 | La1 | C130 | C131 | 136.1 (4) | . | . | . | . | no |
| O13 | La1 | C130 | C131 | -158.5 (4) | . | . | . | . | no |
| N11 | La1 | C130 | C131 | -21.9 (5) | . | . | . | . | no |
| N12 | La1 | C130 | C131 | -76.8 (4) | . | . | . | . | no |
| La1 | O11 | C137 | C138 | 165.4 (3) | . | . | . | . | no |
| C140 | O11 | C137 | C138 | -8.5 (5) | . | . | . | . | no |
| La1 | O11 | C140 | C139 | 171.1 (3) | . | . | . | . | no |
| C137 | O11 | C140 | C139 | -15.4 (5) | . | . | . | . | no |
| C144 | O12 | C141 | C142 | -35.2 (5) | . | . | . | . | no |
| La1 | O12 | C144 | C143 | -163.0 (3) | . | . | . | . | no |
| La1 | O12 | C141 | C142 | 147.6 (3) | . | . | . | . | no |
| C141 | O12 | C144 | C143 | 20.2 (6) | . | . | . | . | no |
| La1 | O13 | C145 | C146 | -167.8 (3) | . | . | . | . | no |
| C148 | O13 | C145 | C146 | 21.4 (5) | . | . | . | . | no |
| C145 | O13 | C148 | C147 | 0.1 (5) | . | . | . | . | no |
| La1 | O13 | C148 | C147 | -172.8 (3) | . | . | . | . | no |
| C34 | O31 | C31 | C32 | 14.4 (12) | . | . | . | . | no |
| C31 | O31 | C34 | C33 | -10.1 (12) | . | . | . | . | no |
| La1 | N11 | C11 | C16 | 81.5 (4) | . | . | . | . | no |
| C113 | N11 | C11 | C12 | 111.8 (5) | . | . | . | . | no |
| C113 | N11 | C11 | C16 | -78.6 (5) | . | . | . | . | no |
| La1 | N11 | C113 | N12 | -3.3 (3) | . | . | . | . | no |
| La1 | N11 | C11 | C12 | -88.1 (4) | . | . | . | . | no |
| C11 | N11 | C113 | C114 | -25.1 (6) | . | . | . | . | no |
| La1 | N11 | C113 | C114 | 170.5 (3) | . | . | . | . | no |
| C11 | N11 | C113 | N12 | 161.1 (4) | . | . | . | . | no |
| C118 | N12 | C113 | N11 | -177.3 (4) | . | . | . | . | no |
| C113 | N12 | C118 | C119 | 78.5 (6) | . | . | . | . | no |
| La1 | N12 | C118 | C119 | -102.2 (4) | . | . | . | . | no |
| La1 | N12 | C113 | C114 | -170.4 (3) | . | . | . | . | no |
| C118 | N12 | C113 | C114 | 9.2 (7) | . | . | . | . | no |
| C113 | N12 | C118 | C123 | -109.9 (5) | . | . | . | . | no |
| La1 | N12 | C113 | N11 | 3.2 (3) | . | . | . | . | no |
| La1 | N12 | C118 | C123 | 69.5 (5) | . | . | . | . | no |
| C12 | C11 | C16 | C110 | 176.1 (4) | . | . | . | . | no |
| C16 | C11 | C12 | C17 | -175.6 (4) | . | . | . | . | no |
| N11 | C11 | C12 | C17 | -6.3 (6) | . | . | . | . | no |
| C16 | C11 | C12 | C13 | 0.9 (6) | . | . | . | . | no |
| C12 | C11 | C16 | C15 | -0.4 (6) | . | . | . | . | no |
| N11 | C11 | C12 | C13 | 170.2 (4) | . | . | . | . | no |
| N11 | C11 | C16 | C110 | 6.4 (6) | . | . | . | . | no |
| N11 | C11 | C16 | C15 | -170.0 (4) | . | . | . | . | no |
| C11 | C12 | C17 | C18 | 104.5 (5) | . | . | . | . | no |
| C11 | C12 | C13 | C14 | -0.9 (6) | . | . | . | . | no |
| C17 | C12 | C13 | C14 | 175.7 (4) | . | . | . | . | no |
| C13 | C12 | C17 | C18 | -71.9 (5) | . | . | . | . | no |
| C11 | C12 | C17 | C19 | -133.0 (4) | . | . | . | . | no |
| C13 | C12 | C17 | C19 | 50.6 (5) | . | . | . | . | no |
| C12 | C13 | C14 | C15 | 0.4 (7) | . | . | . | . | no |
| C13 | C14 | C15 | C16 | 0.2 (6) | . | . | . | . | no |
| C14 | C15 | C16 | C110 | -176.7 (4) | . | . | . | . | no |
| C14 | C15 | C16 | C11 | -0.2 (6) | . | . | . | . | no |

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|------|------|------|-------|------------|---|---|---|---|----|
| C15 | C16 | C110 | C111 | -37.4 (6) | . | . | . | . | no |
| C15 | C16 | C110 | C112 | 86.7 (5) | . | . | . | . | no |
| C11 | C16 | C110 | C111 | 146.2 (4) | . | . | . | . | no |
| C11 | C16 | C110 | C112 | -89.6 (5) | . | . | . | . | no |
| C16 | C110 | C111 | H111 | -50.00 | . | . | . | . | no |
| C112 | C110 | C111 | H111' | 65.00 | . | . | . | . | no |
| H110 | C110 | C111 | H111 | 68.00 | . | . | . | . | no |
| C16 | C110 | C112 | H112' | -179.00 | . | . | . | . | no |
| C16 | C110 | C111 | H111" | 70.00 | . | . | . | . | no |
| C112 | C110 | C111 | H111" | -55.00 | . | . | . | . | no |
| C112 | C110 | C111 | H111 | -175.00 | . | . | . | . | no |
| C16 | C110 | C112 | H112" | 61.00 | . | . | . | . | no |
| C16 | C110 | C111 | H111' | -170.00 | . | . | . | . | no |
| H110 | C110 | C112 | H112' | 64.00 | . | . | . | . | no |
| H110 | C110 | C112 | H112" | -56.00 | . | . | . | . | no |
| H110 | C110 | C112 | H112 | -176.00 | . | . | . | . | no |
| H110 | C110 | C111 | H111' | -52.00 | . | . | . | . | no |
| C16 | C110 | C112 | H112 | -59.00 | . | . | . | . | no |
| C111 | C110 | C112 | H112' | -53.00 | . | . | . | . | no |
| H110 | C110 | C111 | H111" | -171.00 | . | . | . | . | no |
| C111 | C110 | C112 | H112 | 67.00 | . | . | . | . | no |
| C111 | C110 | C112 | H112" | -173.00 | . | . | . | . | no |
| C113 | C114 | C115 | H115' | 67.00 | . | . | . | . | no |
| C117 | C114 | C115 | H115' | -169.00 | . | . | . | . | no |
| C116 | C114 | C115 | H115 | 66.00 | . | . | . | . | no |
| C113 | C114 | C115 | H115 | -173.00 | . | . | . | . | no |
| C117 | C114 | C115 | H115" | 71.00 | . | . | . | . | no |
| C113 | C114 | C115 | H115" | -53.00 | . | . | . | . | no |
| C115 | C114 | C116 | H116' | -179.00 | . | . | . | . | no |
| C115 | C114 | C116 | H116" | 61.00 | . | . | . | . | no |
| C115 | C114 | C116 | H116 | -59.00 | . | . | . | . | no |
| C117 | C114 | C116 | H116' | -65.00 | . | . | . | . | no |
| C117 | C114 | C116 | H116" | 175.00 | . | . | . | . | no |
| C117 | C114 | C116 | H116 | 55.00 | . | . | . | . | no |
| C113 | C114 | C117 | H117' | -63.00 | . | . | . | . | no |
| C113 | C114 | C117 | H117" | 178.00 | . | . | . | . | no |
| C113 | C114 | C117 | H117 | 57.00 | . | . | . | . | no |
| C115 | C114 | C117 | H117' | 179.00 | . | . | . | . | no |
| C115 | C114 | C117 | H117" | 59.00 | . | . | . | . | no |
| C115 | C114 | C117 | H117 | -61.00 | . | . | . | . | no |
| C116 | C114 | C117 | H117' | 63.00 | . | . | . | . | no |
| C116 | C114 | C117 | H117" | -57.00 | . | . | . | . | no |
| C116 | C114 | C117 | H117 | -177.00 | . | . | . | . | no |
| C113 | C114 | C116 | H116 | -178.00 | . | . | . | . | no |
| C116 | C114 | C115 | H115" | -174.00 | . | . | . | . | no |
| C117 | C114 | C115 | H115 | -49.00 | . | . | . | . | no |
| C113 | C114 | C116 | H116' | 62.00 | . | . | . | . | no |
| C116 | C114 | C115 | H115' | -54.00 | . | . | . | . | no |
| C113 | C114 | C116 | H116" | -58.00 | . | . | . | . | no |
| C120 | C119 | C124 | H124 | 158.00 | . | . | . | . | no |
| C118 | C119 | C124 | H124 | -24.00 | . | . | . | . | no |
| C118 | C119 | C120 | H120 | -179.00 | . | . | . | . | no |
| C124 | C119 | C120 | H120 | -1.00 | . | . | . | . | no |
| C119 | C120 | C121 | H121 | -179.00 | . | . | . | . | no |
| H120 | C120 | C121 | H121 | 1.00 | . | . | . | . | no |
| H120 | C120 | C121 | C122 | -179.00 | . | . | . | . | no |
| H121 | C121 | C122 | C123 | 178.00 | . | . | . | . | no |
| C120 | C121 | C122 | H122 | 178.00 | . | . | . | . | no |
| H121 | C121 | C122 | H122 | -2.00 | . | . | . | . | no |
| B2 | C21 | C22 | C23 | -179.8 (4) | . | . | . | . | no |
| C22 | C21 | C26 | C25 | 1.6 (6) | . | . | . | . | no |

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|------|------|------|-------|------------|---|---|---|---|----|
| B2 | C21 | C26 | C25 | -179.5 (4) | . | . | . | . | no |
| C22 | C21 | B2 | C27 | 57.3 (5) | . | . | . | . | no |
| C22 | C21 | B2 | C213 | 177.9 (4) | . | . | . | . | no |
| C22 | C21 | B2 | C219 | -62.3 (5) | . | . | . | . | no |
| C26 | C21 | B2 | C27 | -121.6 (5) | . | . | . | . | no |
| C26 | C21 | B2 | C213 | -1.1 (6) | . | . | . | . | no |
| C26 | C21 | B2 | C219 | 118.8 (5) | . | . | . | . | no |
| C26 | C21 | C22 | C23 | -0.8 (6) | . | . | . | . | no |
| C21 | C22 | C23 | C24 | -0.3 (7) | . | . | . | . | no |
| H122 | C122 | C123 | C118 | -179.00 | . | . | . | . | no |
| H122 | C122 | C123 | C127 | 1.00 | . | . | . | . | no |
| C118 | C123 | C127 | H127 | -9.00 | . | . | . | . | no |
| C122 | C123 | C127 | H127 | 171.00 | . | . | . | . | no |
| C22 | C23 | C24 | C25 | 0.7 (6) | . | . | . | . | no |
| H124 | C124 | C126 | H126' | -61.00 | . | . | . | . | no |
| H124 | C124 | C126 | H126" | 179.00 | . | . | . | . | no |
| C125 | C124 | C126 | H126 | 175.00 | . | . | . | . | no |
| C126 | C124 | C125 | H125' | -62.00 | . | . | . | . | no |
| C126 | C124 | C125 | H125" | 178.00 | . | . | . | . | no |
| C126 | C124 | C125 | H125 | 58.00 | . | . | . | . | no |
| H124 | C124 | C125 | H125' | 54.00 | . | . | . | . | no |
| H124 | C124 | C125 | H125" | -66.00 | . | . | . | . | no |
| H124 | C124 | C125 | H125 | 174.00 | . | . | . | . | no |
| C119 | C124 | C125 | H125 | -68.00 | . | . | . | . | no |
| C125 | C124 | C126 | H126" | -65.00 | . | . | . | . | no |
| C119 | C124 | C126 | H126 | -57.00 | . | . | . | . | no |
| C125 | C124 | C126 | H126' | 55.00 | . | . | . | . | no |
| C23 | C24 | C25 | C26 | 0.1 (7) | . | . | . | . | no |
| H124 | C124 | C126 | H126 | 59.00 | . | . | . | . | no |
| C119 | C124 | C126 | H126" | 63.00 | . | . | . | . | no |
| C119 | C124 | C125 | H125' | 172.00 | . | . | . | . | no |
| C119 | C124 | C126 | H126' | -177.00 | . | . | . | . | no |
| C119 | C124 | C125 | H125" | 52.00 | . | . | . | . | no |
| C24 | C25 | C26 | C21 | -1.3 (7) | . | . | . | . | no |
| C123 | C127 | C128 | H128" | 51.00 | . | . | . | . | no |
| H127 | C127 | C128 | H128' | 52.00 | . | . | . | . | no |
| C123 | C127 | C128 | H128' | 171.00 | . | . | . | . | no |
| H127 | C127 | C128 | H128 | 172.00 | . | . | . | . | no |
| C123 | C127 | C128 | H128 | -69.00 | . | . | . | . | no |
| C129 | C127 | C128 | H128' | -65.00 | . | . | . | . | no |
| C123 | C127 | C129 | H129 | -56.00 | . | . | . | . | no |
| C128 | C127 | C129 | H129' | 59.00 | . | . | . | . | no |
| C128 | C127 | C129 | H129" | -61.00 | . | . | . | . | no |
| H127 | C127 | C128 | H128" | -68.00 | . | . | . | . | no |
| C212 | C27 | C28 | C29 | 2.3 (8) | . | . | . | . | no |
| B2 | C27 | C28 | C29 | -174.1 (5) | . | . | . | . | no |
| C28 | C27 | B2 | C21 | -158.7 (5) | . | . | . | . | no |
| C28 | C27 | B2 | C213 | 77.7 (6) | . | . | . | . | no |
| C129 | C127 | C128 | H128" | 175.00 | . | . | . | . | no |
| C129 | C127 | C128 | H128 | 55.00 | . | . | . | . | no |
| C212 | C27 | B2 | C213 | -98.5 (5) | . | . | . | . | no |
| C212 | C27 | B2 | C219 | 142.5 (5) | . | . | . | . | no |
| C128 | C127 | C129 | H129 | 179.00 | . | . | . | . | no |
| H127 | C127 | C129 | H129' | -58.00 | . | . | . | . | no |
| C123 | C127 | C129 | H129' | -176.00 | . | . | . | . | no |
| C123 | C127 | C129 | H129" | 64.00 | . | . | . | . | no |
| C28 | C27 | C212 | C211 | -1.9 (8) | . | . | . | . | no |
| B2 | C27 | C212 | C211 | 174.5 (5) | . | . | . | . | no |
| H127 | C127 | C129 | H129" | -178.00 | . | . | . | . | no |
| H127 | C127 | C129 | H129 | 62.00 | . | . | . | . | no |
| C28 | C27 | B2 | C219 | -41.4 (6) | . | . | . | . | no |

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|-------|------|------|-------|----------|---|---|---|---|----|
| C212 | C27 | B2 | C21 | 25.2 (7) | . | . | . | . | no |
| C27 | C28 | C29 | C210 | -0.8 (9) | . | . | . | . | no |
| C28 | C29 | C210 | C211 | -1.3 (9) | . | . | . | . | no |
| H130 | C130 | C131 | C132 | 125.00 | . | . | . | . | no |
| H130' | C130 | C131 | C132 | 14.00 | . | . | . | . | no |
| H130 | C130 | C131 | C136 | -56.00 | . | . | . | . | no |
| H130' | C130 | C131 | C136 | -167.00 | . | . | . | . | no |
| C136 | C131 | C132 | H132 | 180.00 | . | . | . | . | no |
| C130 | C131 | C136 | H136 | 0.00 | . | . | . | . | no |
| C130 | C131 | C132 | H132 | -1.00 | . | . | . | . | no |
| C132 | C131 | C136 | H136 | 179.00 | . | . | . | . | no |
| C131 | C132 | C133 | H133 | -179.00 | . | . | . | . | no |
| H132 | C132 | C133 | H133 | 1.00 | . | . | . | . | no |
| H132 | C132 | C133 | C134 | -179.00 | . | . | . | . | no |
| C132 | C133 | C134 | H134 | 179.00 | . | . | . | . | no |
| H133 | C133 | C134 | C135 | 179.00 | . | . | . | . | no |
| H133 | C133 | C134 | H134 | -1.00 | . | . | . | . | no |
| C133 | C134 | C135 | H135 | -180.00 | . | . | . | . | no |
| H134 | C134 | C135 | C136 | -180.00 | . | . | . | . | no |
| H134 | C134 | C135 | H135 | 0.00 | . | . | . | . | no |
| H135 | C135 | C136 | C131 | -180.00 | . | . | . | . | no |
| H135 | C135 | C136 | H136 | 0.00 | . | . | . | . | no |
| C134 | C135 | C136 | H136 | -180.00 | . | . | . | . | no |
| O11 | C137 | C138 | H138' | -90.00 | . | . | . | . | no |
| O11 | C137 | C138 | H138 | 149.00 | . | . | . | . | no |
| H137' | C137 | C138 | C139 | -90.00 | . | . | . | . | no |
| H137 | C137 | C138 | H138' | 30.00 | . | . | . | . | no |
| H137 | C137 | C138 | H138 | -92.00 | . | . | . | . | no |
| H137' | C137 | C138 | H138' | 151.00 | . | . | . | . | no |
| H137' | C137 | C138 | H138 | 30.00 | . | . | . | . | no |
| H137 | C137 | C138 | C139 | 149.00 | . | . | . | . | no |
| H138 | C138 | C139 | C140 | -158.00 | . | . | . | . | no |
| C137 | C138 | C139 | H139 | -157.00 | . | . | . | . | no |
| C137 | C138 | C139 | H139' | 80.00 | . | . | . | . | no |
| H138 | C138 | C139 | H139 | 83.00 | . | . | . | . | no |
| H138' | C138 | C139 | H139 | -38.00 | . | . | . | . | no |
| H138' | C138 | C139 | C140 | 81.00 | . | . | . | . | no |
| H138 | C138 | C139 | H139' | -39.00 | . | . | . | . | no |
| H138' | C138 | C139 | H139' | -160.00 | . | . | . | . | no |
| H139 | C139 | C140 | H140 | -88.00 | . | . | . | . | no |
| C138 | C139 | C140 | H140 | 153.00 | . | . | . | . | no |
| C138 | C139 | C140 | H140' | -86.00 | . | . | . | . | no |
| H139' | C139 | C140 | H140 | 34.00 | . | . | . | . | no |
| H139 | C139 | C140 | O11 | 152.00 | . | . | . | . | no |
| H139' | C139 | C140 | O11 | -86.00 | . | . | . | . | no |
| H139 | C139 | C140 | H140' | 33.00 | . | . | . | . | no |
| H139' | C139 | C140 | H140' | 155.00 | . | . | . | . | no |
| H141 | C141 | C142 | H142 | 37.00 | . | . | . | . | no |
| O12 | C141 | C142 | H142 | -83.00 | . | . | . | . | no |
| H141' | C141 | C142 | C143 | -83.00 | . | . | . | . | no |
| O12 | C141 | C142 | H142' | 155.00 | . | . | . | . | no |
| H141' | C141 | C142 | H142' | 36.00 | . | . | . | . | no |
| H141 | C141 | C142 | C143 | 156.00 | . | . | . | . | no |
| H141 | C141 | C142 | H142' | -85.00 | . | . | . | . | no |
| H141' | C141 | C142 | H142 | 158.00 | . | . | . | . | no |
| C141 | C142 | C143 | H143 | 96.00 | . | . | . | . | no |
| C141 | C142 | C143 | H143' | -143.00 | . | . | . | . | no |
| H142 | C142 | C143 | C144 | 95.00 | . | . | . | . | no |
| H142 | C142 | C143 | H143' | -24.00 | . | . | . | . | no |
| H142' | C142 | C143 | C144 | -143.00 | . | . | . | . | no |
| H142' | C142 | C143 | H143 | -23.00 | . | . | . | . | no |

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|-------|------|------|-------|-----------|---|---|---|---|----|
| H142 | C142 | C143 | H143 | -145.00 | . | . | . | . | no |
| H142' | C142 | C143 | H143' | 98.00 | . | . | . | . | no |
| H143 | C143 | C144 | O12 | -117.00 | . | . | . | . | no |
| H143' | C143 | C144 | O12 | 123.00 | . | . | . | . | no |
| C142 | C143 | C144 | H144' | -118.00 | . | . | . | . | no |
| C142 | C143 | C144 | H144 | 123.00 | . | . | . | . | no |
| H143' | C143 | C144 | H144' | 2.00 | . | . | . | . | no |
| H143 | C143 | C144 | H144' | 123.00 | . | . | . | . | no |
| H143 | C143 | C144 | H144 | 4.00 | . | . | . | . | no |
| H143' | C143 | C144 | H144 | -117.00 | . | . | . | . | no |
| O13 | C145 | C146 | H146' | 85.00 | . | . | . | . | no |
| O13 | C145 | C146 | H146 | -154.00 | . | . | . | . | no |
| H145' | C145 | C146 | H146' | -35.00 | . | . | . | . | no |
| H145 | C145 | C146 | C147 | 85.00 | . | . | . | . | no |
| H145' | C145 | C146 | C147 | -154.00 | . | . | . | . | no |
| H145 | C145 | C146 | H146' | -156.00 | . | . | . | . | no |
| H145 | C145 | C146 | H146 | -34.00 | . | . | . | . | no |
| H145' | C145 | C146 | H146 | 87.00 | . | . | . | . | no |
| C145 | C146 | C147 | H147 | -85.00 | . | . | . | . | no |
| H146' | C146 | C147 | C148 | -85.00 | . | . | . | . | no |
| C145 | C146 | C147 | H147' | 154.00 | . | . | . | . | no |
| H146' | C146 | C147 | H147' | 35.00 | . | . | . | . | no |
| H146 | C146 | C147 | C148 | 154.00 | . | . | . | . | no |
| H146 | C146 | C147 | H147' | -87.00 | . | . | . | . | no |
| H146 | C146 | C147 | H147 | 34.00 | . | . | . | . | no |
| H146' | C146 | C147 | H147 | 156.00 | . | . | . | . | no |
| C146 | C147 | C148 | H148' | -141.00 | . | . | . | . | no |
| H147 | C147 | C148 | H148 | -142.00 | . | . | . | . | no |
| H147 | C147 | C148 | O13 | 98.00 | . | . | . | . | no |
| H147 | C147 | C148 | H148' | -22.00 | . | . | . | . | no |
| H147' | C147 | C148 | O13 | -141.00 | . | . | . | . | no |
| C146 | C147 | C148 | H148 | 98.00 | . | . | . | . | no |
| H147' | C147 | C148 | H148' | 99.00 | . | . | . | . | no |
| H147' | C147 | C148 | H148 | -21.00 | . | . | . | . | no |
| C29 | C210 | C211 | C212 | 1.8(9) | . | . | . | . | no |
| C210 | C211 | C212 | C27 | -0.1(9) | . | . | . | . | no |
| C214 | C213 | C218 | C217 | 1.6(6) | . | . | . | . | no |
| C218 | C213 | C214 | C215 | -1.7(6) | . | . | . | . | no |
| C218 | C213 | B2 | C27 | -14.0(6) | . | . | . | . | no |
| C218 | C213 | B2 | C219 | 106.2(4) | . | . | . | . | no |
| C214 | C213 | B2 | C21 | 48.7(5) | . | . | . | . | no |
| B2 | C213 | C218 | C217 | -175.1(4) | . | . | . | . | no |
| C214 | C213 | B2 | C219 | -70.1(5) | . | . | . | . | no |
| B2 | C213 | C214 | C215 | 175.0(4) | . | . | . | . | no |
| C218 | C213 | B2 | C21 | -135.0(4) | . | . | . | . | no |
| C214 | C213 | B2 | C27 | 169.6(4) | . | . | . | . | no |
| C213 | C214 | C215 | C216 | 0.7(7) | . | . | . | . | no |
| C214 | C215 | C216 | C217 | 0.5(7) | . | . | . | . | no |
| C215 | C216 | C217 | C218 | -0.6(8) | . | . | . | . | no |
| C216 | C217 | C218 | C213 | -0.5(7) | . | . | . | . | no |
| B2 | C219 | C224 | C223 | -177.4(5) | . | . | . | . | no |
| B2 | C219 | C220 | C221 | 176.5(5) | . | . | . | . | no |
| C220 | C219 | C224 | C223 | -1.0(7) | . | . | . | . | no |
| C220 | C219 | B2 | C21 | -89.9(5) | . | . | . | . | no |
| C220 | C219 | B2 | C27 | 151.7(5) | . | . | . | . | no |
| C224 | C219 | B2 | C21 | 86.2(5) | . | . | . | . | no |
| C224 | C219 | C220 | C221 | 0.2(7) | . | . | . | . | no |
| C224 | C219 | B2 | C213 | -151.0(4) | . | . | . | . | no |
| C220 | C219 | B2 | C213 | 32.9(6) | . | . | . | . | no |
| C224 | C219 | B2 | C27 | -32.3(6) | . | . | . | . | no |
| C219 | C220 | C221 | C222 | 1.1(8) | . | . | . | . | no |

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|------|------|------|------|-----------|---|---|---|---|----|
| C220 | C221 | C222 | C223 | -1.6(8) | . | . | . | . | no |
| C221 | C222 | C223 | C224 | 0.8(8) | . | . | . | . | no |
| C222 | C223 | C224 | C219 | 0.5(8) | . | . | . | . | no |
| O31 | C31 | C32 | C33 | -13.9(16) | . | . | . | . | no |
| C31 | C32 | C33 | C34 | 7.9(17) | . | . | . | . | no |
| C32 | C33 | C34 | O31 | 0.9(15) | . | . | . | . | 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

| | | | | | | | | |
|-----|-------|----------|---|---|-------|---|---|----|
| La1 | C17 | 4.452(4) | . | . | . | . | . | no |
| La1 | C18 | 4.455(5) | . | . | . | . | . | no |
| La1 | C110 | 4.216(5) | . | . | . | . | . | no |
| La1 | C112 | 3.810(5) | . | . | . | . | . | no |
| La1 | C126 | 4.551(5) | . | . | . | . | . | no |
| La1 | C127 | 4.192(5) | . | . | . | . | . | no |
| La1 | H112" | 2.8800 | . | . | . | . | . | no |
| La1 | H17 | 3.9500 | . | . | . | . | . | no |
| La1 | H18 | 3.6600 | . | . | . | . | . | no |
| La1 | H110 | 3.9000 | . | . | . | . | . | no |
| La1 | H126 | 3.6600 | . | . | . | . | . | no |
| La1 | H127 | 3.4000 | . | . | . | . | . | no |
| O11 | O12 | 3.062(4) | . | . | . | . | . | no |
| O11 | C144 | 3.198(7) | . | . | . | . | . | no |
| O12 | O13 | 3.009(4) | . | . | . | . | . | no |
| O12 | C148 | 3.393(6) | . | . | . | . | . | no |
| O12 | O11 | 3.062(4) | . | . | . | . | . | no |
| O13 | O12 | 3.009(4) | . | . | . | . | . | no |
| O13 | C130 | 3.347(6) | . | . | . | . | . | no |
| O13 | C141 | 3.228(6) | . | . | . | . | . | no |
| O11 | H144' | 2.5600 | . | . | . | . | . | no |
| O11 | H18 | 2.5300 | . | . | . | . | . | no |
| O12 | H112" | 2.7300 | . | . | . | . | . | no |
| O12 | H148' | 2.8300 | . | . | . | . | . | no |
| O31 | H126' | 2.6600 | . | . | 4_554 | . | . | no |
| N11 | N12 | 2.213(5) | . | . | . | . | . | no |
| N12 | N11 | 2.213(5) | . | . | . | . | . | no |
| N11 | H115' | 2.7800 | . | . | . | . | . | no |
| N11 | H110 | 2.5000 | . | . | . | . | . | no |
| N11 | H116" | 2.9200 | . | . | . | . | . | no |
| N11 | H17 | 2.5200 | . | . | . | . | . | no |
| N12 | H124 | 2.5000 | . | . | . | . | . | no |
| N12 | H127 | 2.4200 | . | . | . | . | . | no |
| N12 | H117 | 2.9100 | . | . | . | . | . | no |
| C11 | C116 | 3.193(6) | . | . | . | . | . | no |
| C11 | C140 | 3.508(7) | . | . | . | . | . | no |
| C11 | C115 | 3.307(6) | . | . | . | . | . | no |
| C12 | C115 | 3.529(6) | . | . | . | . | . | no |
| C16 | C140 | 3.586(7) | . | . | . | . | . | no |
| C16 | C116 | 3.322(6) | . | . | . | . | . | no |
| C17 | La1 | 4.452(4) | . | . | . | . | . | no |
| C17 | C115 | 3.411(6) | . | . | . | . | . | no |
| C18 | La1 | 4.455(5) | . | . | . | . | . | no |
| C22 | C224 | 3.414(8) | . | . | . | . | . | no |
| C22 | C138 | 3.437(8) | . | . | 3_666 | . | . | no |
| C22 | C212 | 3.268(7) | . | . | . | . | . | no |
| C23 | C138 | 3.573(8) | . | . | 3_666 | . | . | no |

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|------|-------|-----------|---|-------|----|
| C24 | C216 | 3.565 (8) | . | 2_655 | no |
| C24 | C144 | 3.559 (8) | . | 3_666 | no |
| C26 | C142 | 3.564 (7) | . | 4_554 | no |
| C26 | C214 | 3.189 (7) | . | . | no |
| C28 | C218 | 3.276 (7) | . | . | no |
| C28 | C224 | 3.161 (8) | . | . | no |
| C110 | La1 | 4.216 (5) | . | . | no |
| C110 | C113 | 3.320 (6) | . | . | no |
| C110 | C116 | 3.377 (6) | . | . | no |
| C11 | H115' | 2.7000 | . | . | no |
| C11 | H140 | 2.6800 | . | . | no |
| C11 | H116" | 2.5200 | . | . | no |
| C12 | H140 | 2.8100 | . | . | no |
| C112 | C140 | 3.597 (8) | . | . | no |
| C12 | H115' | 2.6700 | . | . | no |
| C112 | La1 | 3.810 (5) | . | . | no |
| C13 | H18" | 2.9000 | . | . | no |
| C113 | C124 | 3.359 (6) | . | . | no |
| C113 | C110 | 3.320 (6) | . | . | no |
| C13 | H19 | 2.8000 | . | . | no |
| C13 | H140 | 2.9500 | . | . | no |
| C14 | H140 | 2.9900 | . | . | no |
| C15 | H111 | 2.9900 | . | . | no |
| C15 | H112 | 3.0700 | . | . | no |
| C15 | H125 | 3.0200 | . | 4_554 | no |
| C15 | H111" | 2.8100 | . | . | no |
| C15 | H140 | 2.8600 | . | . | no |
| C115 | C11 | 3.307 (6) | . | . | no |
| C115 | C12 | 3.529 (6) | . | . | no |
| C115 | C17 | 3.411 (6) | . | . | no |
| C116 | C16 | 3.322 (6) | . | . | no |
| C116 | C110 | 3.377 (6) | . | . | no |
| C16 | H140 | 2.7200 | . | . | no |
| C116 | C11 | 3.193 (6) | . | . | no |
| C16 | H116" | 2.5400 | . | . | no |
| C17 | H115' | 2.6600 | . | . | no |
| C117 | C123 | 3.479 (6) | . | . | no |
| C117 | C119 | 3.217 (6) | . | . | no |
| C117 | C118 | 2.862 (6) | . | . | no |
| C117 | C124 | 3.579 (7) | . | . | no |
| C118 | C145 | 3.444 (6) | . | . | no |
| C18 | H137' | 3.0900 | . | . | no |
| C18 | H13 | 3.1000 | . | . | no |
| C118 | C117 | 2.862 (6) | . | . | no |
| C19 | H13 | 2.7700 | . | . | no |
| C119 | C117 | 3.217 (6) | . | . | no |
| C19 | H115' | 2.8600 | . | . | no |
| C21 | H142' | 3.0700 | . | 4_554 | no |
| C121 | C121 | 3.575 (6) | . | 3_567 | no |
| C121 | C122 | 3.554 (6) | . | 3_567 | no |
| C21 | H212 | 2.6400 | . | . | no |
| C21 | H214 | 3.0000 | . | . | no |
| C22 | H138' | 2.9700 | . | 3_666 | no |
| C22 | H138 | 3.0600 | . | 3_666 | no |
| C22 | H212 | 2.8300 | . | . | no |
| C122 | C121 | 3.554 (6) | . | 3_567 | no |
| C123 | C145 | 3.565 (6) | . | . | no |
| C123 | C117 | 3.479 (6) | . | . | no |
| C23 | H138' | 2.8000 | . | 3_666 | no |
| C24 | H216 | 3.0800 | . | 2_655 | no |
| C24 | H33' | 3.0400 | . | . | no |

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|------|-------|-----------|---|-------|----|
| C124 | C113 | 3.359 (6) | . | . | no |
| C24 | H144 | 2.9300 | . | 3_666 | no |
| C124 | C117 | 3.579 (7) | . | . | no |
| C25 | H137 | 3.0500 | . | 3_666 | no |
| C25 | H216 | 3.0600 | . | 2_655 | no |
| C26 | H214 | 2.7500 | . | . | no |
| C126 | La1 | 4.551 (5) | . | . | no |
| C26 | H142' | 2.7100 | . | 4_554 | no |
| C27 | H218 | 2.5500 | . | . | no |
| C27 | H22 | 2.9300 | . | . | no |
| C27 | H224 | 2.7000 | . | . | no |
| C127 | La1 | 4.192 (5) | . | . | no |
| C28 | H224 | 2.7600 | . | . | no |
| C28 | H218 | 2.6100 | . | . | no |
| C29 | H216 | 3.1000 | . | 3_656 | no |
| C130 | O13 | 3.347 (6) | . | . | no |
| C130 | C148 | 3.439 (7) | . | . | no |
| C137 | C144 | 3.523 (9) | . | . | no |
| C138 | C22 | 3.437 (8) | . | 3_666 | no |
| C138 | C23 | 3.573 (8) | . | 3_666 | no |
| C140 | C11 | 3.508 (7) | . | . | no |
| C140 | C112 | 3.597 (8) | . | . | no |
| C140 | C16 | 3.586 (7) | . | . | no |
| C142 | C26 | 3.564 (7) | . | 4_555 | no |
| C144 | C137 | 3.523 (9) | . | . | no |
| C144 | C24 | 3.559 (8) | . | 3_666 | no |
| C145 | C118 | 3.444 (6) | . | . | no |
| C145 | C123 | 3.565 (6) | . | . | no |
| C147 | C216 | 3.573 (8) | . | 2_656 | no |
| C110 | H116' | 3.0600 | . | . | no |
| C110 | H116" | 2.9100 | . | . | no |
| C111 | H15 | 2.6400 | . | . | no |
| C212 | C22 | 3.268 (7) | . | . | no |
| C113 | H110 | 2.5600 | . | . | no |
| C113 | H124 | 2.5900 | . | . | no |
| C114 | H124 | 2.9500 | . | . | no |
| C214 | C26 | 3.189 (7) | . | . | no |
| C214 | C220 | 3.218 (7) | . | . | no |
| C115 | H17 | 2.8000 | . | . | no |
| C115 | H19" | 3.0600 | . | . | no |
| C116 | H110 | 2.7800 | . | . | no |
| C216 | C147 | 3.573 (8) | . | 2_646 | no |
| C116 | H124 | 2.9900 | . | . | no |
| C216 | C24 | 3.565 (8) | . | 2_645 | no |
| C117 | H121 | 2.9600 | . | 3_567 | no |
| C118 | H145' | 2.6300 | . | . | no |
| C218 | C28 | 3.276 (7) | . | . | no |
| C118 | H117 | 2.5800 | . | . | no |
| C118 | H117' | 2.5700 | . | . | no |
| C119 | H145' | 2.8000 | . | . | no |
| C119 | H117' | 2.5000 | . | . | no |
| C120 | H126" | 3.0500 | . | . | no |
| C120 | H125" | 3.0400 | . | . | no |
| C120 | H145' | 2.9900 | . | . | no |
| C120 | H125 | 2.7900 | . | . | no |
| C220 | C214 | 3.218 (7) | . | . | no |
| C121 | H145' | 3.0600 | . | . | no |
| C122 | H145' | 2.9300 | . | . | no |
| C122 | H128 | 2.8300 | . | . | no |
| C122 | H134 | 3.0300 | . | 4_565 | no |
| C122 | H129" | 2.9400 | . | . | no |

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|------|-------|-----------|---|-------|----|
| C123 | H117 | 2.8200 | . | . | no |
| C123 | H145' | 2.7100 | . | . | no |
| C124 | H110 | 3.0600 | . | . | no |
| C224 | C22 | 3.414 (8) | . | . | no |
| C124 | H117' | 2.7600 | . | . | no |
| C224 | C28 | 3.161 (8) | . | . | no |
| C125 | H117' | 3.0700 | . | . | no |
| C125 | H120 | 2.6600 | . | . | no |
| C126 | H141 | 3.0300 | . | . | no |
| C127 | H136 | 2.9800 | . | . | no |
| C128 | H221 | 3.0300 | . | 2_656 | no |
| C128 | H130 | 2.8100 | . | . | no |
| C128 | H122 | 2.8200 | . | . | no |
| C129 | H111 | 2.8100 | . | 2_556 | no |
| C129 | H122 | 3.0800 | . | . | no |
| C129 | H117 | 3.0000 | . | . | no |
| C130 | H148 | 2.8900 | . | . | no |
| C130 | H127 | 3.1000 | . | . | no |
| C132 | H214 | 3.0800 | . | 3_666 | no |
| C132 | H137' | 3.0100 | . | . | no |
| C133 | H146' | 2.9400 | . | 4_564 | no |
| C133 | H18' | 3.0900 | . | . | no |
| C134 | H18' | 3.1000 | . | . | no |
| C137 | H144' | 2.8300 | . | . | no |
| C137 | H18 | 2.8000 | . | . | no |
| C138 | H144' | 3.0400 | . | . | no |
| C138 | H23 | 3.0200 | . | . | no |
| C140 | H144' | 2.8400 | . | . | no |
| C140 | H112" | 3.0700 | . | . | no |
| C141 | H145 | 3.0400 | . | . | no |
| C144 | H137 | 3.0500 | . | . | no |
| C146 | H133 | 2.9700 | . | 4_565 | no |
| C148 | H130 | 3.1000 | . | . | no |
| C210 | H112 | 2.7600 | . | . | no |
| C210 | H146 | 3.0000 | . | 4_554 | no |
| C211 | H145 | 3.0400 | . | 4_554 | no |
| C211 | H112 | 3.1000 | . | . | no |
| C213 | H143 | 3.0800 | . | 4_554 | no |
| C213 | H220 | 2.7500 | . | . | no |
| C213 | H26 | 2.7900 | . | . | no |
| C213 | H147' | 3.0900 | . | 2_646 | no |
| C214 | H26 | 2.5400 | . | . | no |
| C214 | H143 | 2.9200 | . | 4_554 | no |
| C214 | H147' | 3.0000 | . | 2_646 | no |
| C214 | H220 | 2.5100 | . | . | no |
| C214 | H132 | 3.0000 | . | 3_666 | no |
| C215 | H143 | 3.0300 | . | 4_554 | no |
| C215 | H147' | 3.0400 | . | 2_646 | no |
| C215 | H223 | 3.0000 | . | 4_554 | no |
| C215 | H133 | 3.0800 | . | 3_666 | no |
| C216 | H24 | 2.8800 | . | 2_645 | no |
| C218 | H141' | 3.1000 | . | 4_554 | no |
| C218 | H147 | 3.0100 | . | 4_554 | no |
| C219 | H138 | 2.8300 | . | 3_666 | no |
| C219 | H22 | 2.9800 | . | . | no |
| C219 | H28 | 2.7900 | . | . | no |
| C220 | H147' | 3.0100 | . | 2_646 | no |
| C220 | H138 | 2.7900 | . | 3_666 | no |
| C220 | H214 | 3.0000 | . | . | no |
| C221 | H148 | 2.9900 | . | 2_646 | no |
| C221 | H138 | 2.9800 | . | 3_666 | no |

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|-------|-------|--------|---|-------|----|
| C224 | H22 | 2.8400 | . | . | no |
| C224 | H23 | 3.0900 | . | 3_666 | no |
| C224 | H138 | 3.0100 | . | 3_666 | no |
| C224 | H28 | 2.8100 | . | . | no |
| H111' | H112' | 2.4800 | . | . | no |
| H111" | H112 | 2.5200 | . | . | no |
| H111" | H15 | 2.2200 | . | . | no |
| H111" | H120 | 2.5400 | . | 4_554 | no |
| H111" | C15 | 2.8100 | . | . | no |
| H112' | H111' | 2.4800 | . | . | no |
| H112" | C140 | 3.0700 | . | . | no |
| H112" | O12 | 2.7300 | . | . | no |
| H112" | La1 | 2.8800 | . | . | no |
| H115' | C12 | 2.6700 | . | . | no |
| H115' | C17 | 2.6600 | . | . | no |
| H115' | C11 | 2.7000 | . | . | no |
| H115' | N11 | 2.7800 | . | . | no |
| H115' | C19 | 2.8600 | . | . | no |
| H115' | H116" | 2.4500 | . | . | no |
| H115' | H19" | 2.2700 | . | . | no |
| H115' | H17 | 2.2800 | . | . | no |
| H115" | H117 | 2.5400 | . | . | no |
| H115" | H17 | 2.5200 | . | . | no |
| H116' | C110 | 3.0600 | . | . | no |
| H116' | H110 | 2.3600 | . | . | no |
| H116' | H117' | 2.5000 | . | . | no |
| H116' | H124 | 2.2900 | . | . | no |
| H116" | C110 | 2.9100 | . | . | no |
| H116" | H115' | 2.4500 | . | . | no |
| H116" | C11 | 2.5200 | . | . | no |
| H116" | C16 | 2.5400 | . | . | no |
| H116" | N11 | 2.9200 | . | . | no |
| H116" | H110 | 2.5800 | . | . | no |
| H117' | C118 | 2.5700 | . | . | no |
| H117' | H125" | 2.5000 | . | . | no |
| H117' | C124 | 2.7600 | . | . | no |
| H117' | C125 | 3.0700 | . | . | no |
| H117' | H116' | 2.5000 | . | . | no |
| H117' | C119 | 2.5000 | . | . | no |
| H117' | H124 | 2.4500 | . | . | no |
| H117" | H115 | 2.3400 | . | . | no |
| H117" | H31 | 2.5400 | . | 3_566 | no |
| H117" | H116 | 2.3800 | . | . | no |
| H125' | H126' | 2.5000 | . | . | no |
| H125" | C120 | 3.0400 | . | . | no |
| H125" | H135 | 2.5100 | . | 2_546 | no |
| H125" | H117' | 2.5000 | . | . | no |
| H13 | C18 | 3.1000 | . | . | no |
| H13 | H19 | 2.2500 | . | . | no |
| H13 | C19 | 2.7700 | . | . | no |
| H126' | O31 | 2.6600 | . | 4_555 | no |
| H126' | H125' | 2.5000 | . | . | no |
| H126" | H15 | 2.4600 | . | 4_555 | no |
| H126" | C120 | 3.0500 | . | . | no |
| H126" | H125 | 2.5500 | . | . | no |
| H15 | H111" | 2.2200 | . | . | no |
| H15 | H126" | 2.4600 | . | 4_554 | no |
| H15 | H125 | 2.4900 | . | 4_554 | no |
| H15 | C111 | 2.6400 | . | . | no |
| H128' | H129' | 2.5400 | . | . | no |
| H128' | H221 | 2.5800 | . | 2_656 | no |

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|-------|-------|--------|---|-------|----|
| H128' | H130 | 2.4900 | . | . | no |
| H128" | H146' | 2.5700 | . | . | no |
| H128" | H130 | 2.5200 | . | . | no |
| H17 | C115 | 2.8000 | . | . | no |
| H17 | H115' | 2.2800 | . | . | no |
| H17 | La1 | 3.9500 | . | . | no |
| H17 | H115" | 2.5200 | . | . | no |
| H17 | N11 | 2.5200 | . | . | no |
| H129' | H128' | 2.5400 | . | . | no |
| H18 | O11 | 2.5300 | . | . | no |
| H18 | C137 | 2.8000 | . | . | no |
| H18 | La1 | 3.6600 | . | . | no |
| H18 | H137' | 2.2700 | . | . | no |
| H18' | C133 | 3.0900 | . | . | no |
| H18' | H19' | 2.4800 | . | . | no |
| H18' | H128 | 2.5800 | . | 4_564 | no |
| H18' | C134 | 3.1000 | . | . | no |
| H18" | H19 | 2.5100 | . | . | no |
| H18" | C13 | 2.9000 | . | . | no |
| H129" | C122 | 2.9400 | . | . | no |
| H129" | H128 | 2.4700 | . | . | no |
| H19 | H13 | 2.2500 | . | . | no |
| H19 | H18" | 2.5100 | . | . | no |
| H19 | C13 | 2.8000 | . | . | no |
| H19' | H18' | 2.4800 | . | . | no |
| H19" | H115' | 2.2700 | . | . | no |
| H19" | C115 | 3.0600 | . | . | no |
| H130' | H132 | 2.2400 | . | . | no |
| H137' | C18 | 3.0900 | . | . | no |
| H137' | C132 | 3.0100 | . | . | no |
| H137' | H132 | 2.5800 | . | . | no |
| H137' | H18 | 2.2700 | . | . | no |
| H138' | H144' | 2.5400 | . | . | no |
| H138' | C22 | 2.9700 | . | 3_666 | no |
| H138' | C23 | 2.8000 | . | 3_666 | no |
| H22 | C27 | 2.9300 | . | . | no |
| H22 | C219 | 2.9800 | . | . | no |
| H22 | H224 | 2.4500 | . | . | no |
| H22 | C224 | 2.8400 | . | . | no |
| H23 | C224 | 3.0900 | . | 3_666 | no |
| H23 | C138 | 3.0200 | . | . | no |
| H140' | H144' | 2.3500 | . | . | no |
| H24 | C216 | 2.8800 | . | 2_655 | no |
| H24 | H216 | 2.5900 | . | 2_655 | no |
| H24 | H144 | 2.5600 | . | 3_666 | no |
| H24 | H223 | 2.5900 | . | 3_666 | no |
| H141' | C218 | 3.1000 | . | 4_555 | no |
| H25 | H216 | 2.5500 | . | 2_655 | no |
| H142' | C26 | 2.7100 | . | 4_555 | no |
| H142' | H212 | 2.4800 | . | 4_555 | no |
| H142' | C21 | 3.0700 | . | 4_555 | no |
| H142' | H26 | 2.5300 | . | 4_555 | no |
| H26 | H214 | 2.1800 | . | . | no |
| H26 | C213 | 2.7900 | . | . | no |
| H26 | C214 | 2.5400 | . | . | no |
| H26 | H142' | 2.5300 | . | 4_554 | no |
| H143' | H224 | 2.3700 | . | . | no |
| H144' | H137 | 2.5400 | . | . | no |
| H144' | C138 | 3.0400 | . | . | no |
| H144' | C140 | 2.8400 | . | . | no |
| H144' | C137 | 2.8300 | . | . | no |

| | | | | | |
|-------|-------|--------|---|-------|----|
| H144' | H140' | 2.3500 | . | . | no |
| H144' | O11 | 2.5600 | . | . | no |
| H144' | H138' | 2.5400 | . | . | no |
| H28 | C219 | 2.7900 | . | . | no |
| H28 | C224 | 2.8100 | . | . | no |
| H145' | C119 | 2.8000 | . | . | no |
| H145' | C118 | 2.6300 | . | . | no |
| H145' | C121 | 3.0600 | . | . | no |
| H145' | C122 | 2.9300 | . | . | no |
| H145' | C120 | 2.9900 | . | . | no |
| H145' | C123 | 2.7100 | . | . | no |
| H29 | H216 | 2.4100 | . | 3_656 | no |
| H146' | C133 | 2.9400 | . | 4_565 | no |
| H146' | H133 | 2.1800 | . | 4_565 | no |
| H146' | H128" | 2.5700 | . | . | no |
| H147' | C214 | 3.0000 | . | 2_656 | no |
| H147' | C215 | 3.0400 | . | 2_656 | no |
| H147' | C213 | 3.0900 | . | 2_656 | no |
| H147' | H220 | 2.5600 | . | 2_656 | no |
| H147' | C220 | 3.0100 | . | 2_656 | no |
| H31 | H117" | 2.5400 | . | 3_566 | no |
| H148' | O12 | 2.8300 | . | . | no |
| H33' | C24 | 3.0400 | . | . | no |
| H110 | La1 | 3.9000 | . | . | no |
| H110 | C124 | 3.0600 | . | . | no |
| H110 | H116' | 2.3600 | . | . | no |
| H110 | H116" | 2.5800 | . | . | no |
| H110 | C116 | 2.7800 | . | . | no |
| H110 | N11 | 2.5000 | . | . | no |
| H110 | C113 | 2.5600 | . | . | no |
| H110 | H124 | 2.1800 | . | . | no |
| H111 | C15 | 2.9900 | . | . | no |
| H111 | C129 | 2.8100 | . | 2_546 | no |
| H111 | H129 | 2.6000 | . | 2_546 | no |
| H112 | C210 | 2.7600 | . | . | no |
| H112 | C211 | 3.1000 | . | . | no |
| H112 | C15 | 3.0700 | . | . | no |
| H112 | H210 | 2.3100 | . | . | no |
| H112 | H111" | 2.5200 | . | . | no |
| H115 | H116 | 2.5300 | . | . | no |
| H115 | H117" | 2.3400 | . | . | no |
| H116 | H115 | 2.5300 | . | . | no |
| H116 | H117" | 2.3800 | . | . | no |
| H117 | C118 | 2.5800 | . | . | no |
| H117 | H129 | 2.1900 | . | . | no |
| H117 | N12 | 2.9100 | . | . | no |
| H117 | C129 | 3.0000 | . | . | no |
| H117 | H115" | 2.5400 | . | . | no |
| H117 | C123 | 2.8200 | . | . | no |
| H117 | H121 | 2.4900 | . | 3_567 | no |
| H120 | H125 | 2.2000 | . | . | no |
| H120 | C125 | 2.6600 | . | . | no |
| H120 | H111" | 2.5400 | . | 4_555 | no |
| H121 | H117 | 2.4900 | . | 3_567 | no |
| H121 | C117 | 2.9600 | . | 3_567 | no |
| H122 | C128 | 2.8200 | . | . | no |
| H122 | H134 | 2.4700 | . | 4_565 | no |
| H122 | H128 | 2.3300 | . | . | no |
| H122 | C129 | 3.0800 | . | . | no |
| H124 | H117' | 2.4500 | . | . | no |
| H124 | C113 | 2.5900 | . | . | no |

| | | | | | |
|------|-------|--------|---|-------|----|
| H124 | N12 | 2.5000 | . | . | no |
| H124 | H110 | 2.1800 | . | . | no |
| H124 | C116 | 2.9900 | . | . | no |
| H124 | H116' | 2.2900 | . | . | no |
| H124 | C114 | 2.9500 | . | . | no |
| H125 | C120 | 2.7900 | . | . | no |
| H125 | H126" | 2.5500 | . | . | no |
| H125 | H15 | 2.4900 | . | 4_555 | no |
| H125 | H120 | 2.2000 | . | . | no |
| H125 | C15 | 3.0200 | . | 4_555 | no |
| H126 | La1 | 3.6600 | . | . | no |
| H126 | H141 | 2.2300 | . | . | no |
| H127 | N12 | 2.4200 | . | . | no |
| H127 | C130 | 3.1000 | . | . | no |
| H127 | La1 | 3.4000 | . | . | no |
| H127 | H136 | 2.2700 | . | . | no |
| H128 | H122 | 2.3300 | . | . | no |
| H128 | C122 | 2.8300 | . | . | no |
| H128 | H129" | 2.4700 | . | . | no |
| H128 | H18' | 2.5800 | . | 4_565 | no |
| H129 | H117 | 2.1900 | . | . | no |
| H129 | H111 | 2.6000 | . | 2_556 | no |
| H130 | H128" | 2.5200 | . | . | no |
| H130 | H148 | 2.4300 | . | . | no |
| H130 | C148 | 3.1000 | . | . | no |
| H130 | H128' | 2.4900 | . | . | no |
| H130 | C128 | 2.8100 | . | . | no |
| H132 | C214 | 3.0000 | . | 3_666 | no |
| H132 | H137' | 2.5800 | . | . | no |
| H132 | H214 | 2.2500 | . | 3_666 | no |
| H132 | H130' | 2.2400 | . | . | no |
| H133 | C146 | 2.9700 | . | 4_564 | no |
| H133 | H146' | 2.1800 | . | 4_564 | no |
| H133 | C215 | 3.0800 | . | 3_666 | no |
| H134 | H122 | 2.4700 | . | 4_564 | no |
| H134 | C122 | 3.0300 | . | 4_564 | no |
| H135 | H125" | 2.5100 | . | 2_556 | no |
| H136 | H127 | 2.2700 | . | . | no |
| H136 | C127 | 2.9800 | . | . | no |
| H137 | C144 | 3.0500 | . | . | no |
| H137 | H144' | 2.5400 | . | . | no |
| H137 | C25 | 3.0500 | . | 3_666 | no |
| H138 | C219 | 2.8300 | . | 3_666 | no |
| H138 | C224 | 3.0100 | . | 3_666 | no |
| H138 | C22 | 3.0600 | . | 3_666 | no |
| H138 | C220 | 2.7900 | . | 3_666 | no |
| H138 | C221 | 2.9800 | . | 3_666 | no |
| H140 | C15 | 2.8600 | . | . | no |
| H140 | C11 | 2.6800 | . | . | no |
| H140 | C14 | 2.9900 | . | . | no |
| H140 | C12 | 2.8100 | . | . | no |
| H140 | C13 | 2.9500 | . | . | no |
| H140 | C16 | 2.7200 | . | . | no |
| H141 | H126 | 2.2300 | . | . | no |
| H141 | C126 | 3.0300 | . | . | no |
| H143 | C215 | 3.0300 | . | 4_555 | no |
| H143 | C213 | 3.0800 | . | 4_555 | no |
| H143 | C214 | 2.9200 | . | 4_555 | no |
| H144 | C24 | 2.9300 | . | 3_666 | no |
| H144 | H24 | 2.5600 | . | 3_666 | no |
| H145 | C211 | 3.0400 | . | 4_555 | no |

| | | | | | |
|------|-------|--------|---|-------|----|
| H145 | C141 | 3.0400 | . | . | no |
| H146 | C210 | 3.0000 | . | 4_555 | no |
| H147 | H218 | 2.2800 | . | 4_555 | no |
| H147 | C218 | 3.0100 | . | 4_555 | no |
| H148 | C221 | 2.9900 | . | 2_656 | no |
| H148 | C130 | 2.8900 | . | . | no |
| H148 | H130 | 2.4300 | . | . | no |
| H210 | H112 | 2.3100 | . | . | no |
| H212 | C21 | 2.6400 | . | . | no |
| H212 | C22 | 2.8300 | . | . | no |
| H212 | H142' | 2.4800 | . | 4_554 | no |
| H214 | H26 | 2.1800 | . | . | no |
| H214 | H220 | 2.2600 | . | . | no |
| H214 | C220 | 3.0000 | . | . | no |
| H214 | H132 | 2.2500 | . | 3_666 | no |
| H214 | C26 | 2.7500 | . | . | no |
| H214 | C132 | 3.0800 | . | 3_666 | no |
| H214 | C21 | 3.0000 | . | . | no |
| H215 | H223 | 2.5100 | . | 4_554 | no |
| H216 | H25 | 2.5500 | . | 2_645 | no |
| H216 | C29 | 3.1000 | . | 3_656 | no |
| H216 | H29 | 2.4100 | . | 3_656 | no |
| H216 | H24 | 2.5900 | . | 2_645 | no |
| H216 | C24 | 3.0800 | . | 2_645 | no |
| H216 | C25 | 3.0600 | . | 2_645 | no |
| H218 | C27 | 2.5500 | . | . | no |
| H218 | H147 | 2.2800 | . | 4_554 | no |
| H218 | C28 | 2.6100 | . | . | no |
| H220 | H214 | 2.2600 | . | . | no |
| H220 | C214 | 2.5100 | . | . | no |
| H220 | C213 | 2.7500 | . | . | no |
| H220 | H147' | 2.5600 | . | 2_646 | no |
| H221 | C128 | 3.0300 | . | 2_646 | no |
| H221 | H128' | 2.5800 | . | 2_646 | no |
| H223 | H215 | 2.5100 | . | 4_555 | no |
| H223 | H24 | 2.5900 | . | 3_666 | no |
| H223 | C215 | 3.0000 | . | 4_555 | no |
| H224 | C27 | 2.7000 | . | . | no |
| H224 | C28 | 2.7600 | . | . | no |
| H224 | H22 | 2.4500 | . | . | no |
| H224 | H143' | 2.3700 | . | . | 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)

#

| | | | | | | | | |
|------|-------|-----|--------|--------|----------|--------|---|-----|
| C17 | H17 | N11 | 1.0000 | 2.5200 | 2.964(6) | 107.00 | . | yes |
| C18 | H18 | O11 | 0.9800 | 2.5300 | 3.464(6) | 160.00 | . | yes |
| C144 | H144' | O11 | 0.9900 | 2.5600 | 3.198(7) | 122.00 | . | yes |
| C110 | H110 | N11 | 1.0000 | 2.5000 | 2.886(6) | 102.00 | . | yes |
| C124 | H124 | N12 | 1.0000 | 2.5000 | 2.915(6) | 104.00 | . | yes |
| C127 | H127 | N12 | 1.0000 | 2.4200 | 2.918(6) | 110.00 | . | 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