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

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;

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# 1. SUBMISSION DETAILS

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

_publ_requested_journal         'Organo Metallics'
# Publication choise 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 Metallics
  (Our Compound_Identification_Code : Q1077)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic   ?

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_journal_date_printers_final   ?
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_journal_issue                 ?
_journal_page_first            ?
_journal_page_last             ?

_journal_suppl_publ_number     ?
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3. TITLE AND AUTHOR LIST

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_publ_section_title
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?
;
_publ_section_title_footnote
;
?
;

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# The loop structure below should contain the names and adresses 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., Israel, & Smits, J.M.M. (1999).
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```

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Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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Volume A, Space-group symmetry, Kluwer Academic Publishers,
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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
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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
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#=====

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

_diffn_standards_number         0
_diffn_standards_interval_count ?
_diffn_standards_interval_time  ?
_diffn_standards_decay_%        0

loop_
_diffn_standard_refl_index_h
_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_reflns_number            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

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```

_diffn_reflms_limit_l_min      -23
_diffn_reflms_limit_l_max      23
_diffn_reflms_theta_min        2.26
_diffn_reflms_theta_max        26.37
_diffn_measured_fraction_theta_max  0.998
_diffn_reflms_theta_full       25.00
_diffn_measured_fraction_theta_full  0.999

_diffn_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\sigma(I)

_computing_data_collection      'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement      'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction       'XPREP, Version 5.1/NT, (Bruker, 2000)'
_computing_structure_solution
;
  DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
  PLUTO (Meetsma, 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/[\sigma^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
_vrn_publ_code_void_volume	143.6
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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_z
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_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	. .

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_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22

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_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
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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)

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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

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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_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
O11      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
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

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

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

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

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

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

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

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

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

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

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