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Scandium, Yttrium, and Lanthanum Benzyl and Alkynyl Complexes with the N-(2-Pyrrolidin-1-ylethyl)-1,4-diazepan-6-amido Ligand

Ge, Shaozhong; Meetsma, Auke; Hessen, Bart

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# 1. SUBMISSION DETAILS

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

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

_publ_contact_letter                 # Include date of submission
;
  Date of submission :  2008-12-02  09:01:14

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  X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : q1477)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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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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; # author related footnote
;
; # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote
;
;

```

Crystal Structure Center, Chemical Physics,
Zernike Institute for Advanced Materials,
University of Groningen,
Nijenborgh 4,
NL-9747 AG Groningen, The Netherlands.

;

#=====

4. TEXT

_publ_section_synopsis

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Insert blank lines between paragraphs

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_publ_section_exptl_prep

;

;

_publ_section_exptl_refinement

;

The hydrogen atoms were generated by geometrical considerations,
constrained to idealized geometries, and allowed to ride on the
carrier atom with an isotropic displacement parameter related to the
equivalent displacement parameter of their carrier atoms,
with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(\text{methyl } C)$.

The methyl-groups were refined as rigid groups, which were allowed
to rotate freely.

Assigned values of bond distances: secondary C-H₂ = 0.99 Å,
methyl C-H₃ = 0.98 Å and aromatic C-H = 0.95 Å.

;

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;

;

Insert blank lines between references

_publ_section_references

;

Allen, F.H. (2002). Acta Cryst. B58, 380-388.

Beurskens, P.T., Beurskens, G., Gelder, R. de, Smits, J.M.M.,
García-Granda, S. & Gould, R.O. (2008).

The DIRDIF08 program system, Technical Report of the Crystallography
Laboratory, University of Nijmegen, The Netherlands.

Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

Bruker, (2007). SMART (Version 5.632), SAINT-Plus (Version 7.46a) and
SADABS (Version 2.10). 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.

Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

Meetsma, A. (2008). Extended version of the program PLUTO. University of Groningen, The Netherlands. (unpublished).

Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.

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

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Fig. 1. Perspective PLUTO drawings 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 atoms are represented at the 50% probability level.
The H-atoms have been omitted to improve clarity.

;

_publ_section_acknowledgements

;

;

#=====

5. CHEMICAL DATA

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;

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C60 H78 La2 N8'

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

'C60 H78 La2 N8'

_chemical_formula_iupac ?

_chemical_formula_weight 1189.14

_chemical_compound_source 'see text'

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'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'
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

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_symmetry_space_group_name_H-M 'P 21/n'
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loop_
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_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,1/2-z
3 -x,-y,-z
4 1/2+x,1/2-y,1/2+z

_cell_length_a      13.8365(16)
_cell_length_b      14.4305(16)
_cell_length_c      14.2150(16)
_cell_angle_alpha    90
_cell_angle_beta     92.3806(17)
_cell_angle_gamma    90
_cell_volume         2835.8(6)
_cell_formula_units_Z 2

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 4140
_cell_measurement_theta_min 2.46
_cell_measurement_theta_max 28.64
_cell_special_details

;
The final unit cell was obtained from the xyz centroids of
4140 reflections after integration using the SAINTPLUS
software package (Bruker, 2007).

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

_exptl_crystal_description      'block'
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# 7. EXPERIMENTAL DATA

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;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
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;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2007)).
;
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? ? ?

# number of measured reflections (redundant set)
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_diffn_reflns_av_sigmaI/netI    0.0727
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_diffn_reflns_limit_k_max       17
_diffn_reflns_limit_l_min       -17
_diffn_reflns_limit_l_max       17

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_diffn_refl_theta_full      25.00
_diffn_meas_fraction_theta_full  0.999

_diffn_refl_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
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_refl_number_gt             4139
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DIRDIF-08 (Beurskens et al., 2008)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
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PLATON (Spek, 2003)
PLUTO (Meetsma, 2008)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

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Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on  $F^2$ , conventional R-factors R are based
on F, with F set to zero for negative  $F^2$ . The threshold expression of
 $F^2 > 2\sigma(F^2)$  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.
;

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_refine_ls_weighting_details
'calc w=1/[\sigma^2(Fo^2)+(0.0478P)^2+0.0P] where P=(Fo^2+2Fc^2)/3'
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_refine_ls_R_factor_gt 0.0411
_refine_ls_wR_factor_ref 0.0964
_refine_ls_wR_factor_gt 0.0874
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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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N3 N Uani -0.0847(3) 0.2560(2) 0.1189(2) 1.000 0.0178(11) . .
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 H1'' H Uiso -0.24840 0.06253 0.05802 1.000 0.0406 . .
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 H7' H Uiso -0.18672 0.30406 0.32322 1.000 0.0340 . .
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 H8' H Uiso -0.24833 0.17448 0.17089 1.000 0.0250 . .
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 H9' H Uiso -0.21196 0.31329 0.07844 1.000 0.0230 . .
 H10 H Uiso -0.17359 0.23635 -0.05692 1.000 0.0244 . .
 H10' H Uiso -0.16679 0.34429 -0.08178 1.000 0.0244 . .
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 H11' H Uiso -0.04728 0.19905 -0.18787 1.000 0.0242 . .
 H12 H Uiso 0.08597 0.29896 -0.25540 1.000 0.0324 . .
 H12' H Uiso 0.11652 0.22607 -0.17353 1.000 0.0324 . .
 H13 H Uiso 0.16572 0.35020 -0.08760 1.000 0.0280 . .
 H13' H Uiso 0.10894 0.42094 -0.15779 1.000 0.0280 . .
 H14 H Uiso 0.04662 0.37203 0.01239 1.000 0.0261 . .
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 H26 H Uiso 0.40765 0.09360 -0.02103 1.000 0.0286 . .
 H27 H Uiso 0.57363 0.11003 -0.02401 1.000 0.0411 . .
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N3 0.0183(19) 0.020(2) 0.0152(18) 0.0004(16) 0.0016(15) 0.0006(16)
N4 0.019(2) 0.019(2) 0.0214(19) 0.0012(16) 0.0010(16) -0.0035(17)
C1 0.026(3) 0.026(3) 0.030(3) -0.004(2) 0.008(2) -0.007(2)
C2 0.033(3) 0.018(3) 0.025(2) 0.006(2) 0.009(2) -0.002(2)
C3 0.032(3) 0.023(3) 0.019(2) 0.004(2) 0.003(2) 0.006(2)
C4 0.026(2) 0.030(3) 0.018(2) -0.006(2) -0.0037(19) 0.008(2)
C5 0.025(2) 0.021(3) 0.018(2) -0.006(2) 0.0005(19) 0.002(2)
C6 0.020(2) 0.018(3) 0.017(2) -0.0008(19) 0.0026(19) 0.002(2)
C7 0.024(2) 0.024(3) 0.020(2) -0.002(2) 0.005(2) 0.004(2)
C8 0.019(2) 0.026(3) 0.018(2) -0.0015(19) 0.0056(18) 0.001(2)
C9 0.014(2) 0.021(3) 0.023(2) 0.001(2) -0.0004(18) 0.002(2)
C10 0.017(2) 0.024(3) 0.021(2) 0.003(2) 0.0005(19) 0.005(2)
C11 0.027(2) 0.019(3) 0.015(2) -0.0006(19) 0.0035(19) -0.003(2)
C12 0.028(3) 0.032(3) 0.022(2) 0.003(2) 0.006(2) -0.002(2)
C13 0.022(2) 0.022(3) 0.027(2) 0.006(2) 0.0019(19) -0.002(2)
C14 0.028(2) 0.024(3) 0.013(2) -0.003(2) -0.0006(19) -0.019(2)
C15 0.023(2) 0.017(2) 0.016(2) -0.0008(19) 0.0013(19) -0.001(2)
C16 0.025(2) 0.011(2) 0.014(2) 0.0007(18) 0.0012(19) 0.004(2)
C17 0.021(2) 0.014(2) 0.017(2) -0.0022(18) -0.0001(18) 0.0052(19)
C18 0.024(2) 0.017(3) 0.022(2) 0.003(2) 0.0024(19) 0.002(2)
C19 0.017(2) 0.023(3) 0.028(2) -0.002(2) 0.0007(19) -0.002(2)
C20 0.023(2) 0.020(3) 0.028(2) -0.002(2) -0.011(2) 0.008(2)
C21 0.027(3) 0.024(3) 0.024(2) 0.008(2) -0.008(2) -0.003(2)
C22 0.024(2) 0.020(3) 0.028(2) 0.004(2) -0.001(2) -0.003(2)
C23 0.023(3) 0.016(3) 0.028(2) -0.003(2) 0.001(2) 0.003(2)
C24 0.025(3) 0.018(3) 0.020(2) 0.0011(19) 0.001(2) -0.001(2)
C25 0.019(2) 0.028(3) 0.016(2) 0.005(2) -0.0012(19) -0.003(2)
C26 0.020(2) 0.030(3) 0.022(2) 0.011(2) 0.0013(19) 0.001(2)
C27 0.022(3) 0.053(4) 0.028(3) 0.014(3) 0.004(2) 0.007(3)
C28 0.021(3) 0.072(5) 0.028(3) 0.014(3) -0.001(2) -0.013(3)
C29 0.045(4) 0.051(4) 0.021(3) -0.002(3) -0.002(2) -0.027(3)
C30 0.039(3) 0.033(3) 0.025(3) -0.004(2) 0.008(2) -0.012(3)

#=====

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

La	N1	2.850(4)	.	.	yes
La	N2	2.730(3)	.	.	yes
La	N3	2.339(3)	.	.	yes
La	N4	2.781(4)	.	.	yes

La	C15	2.670(4)	.	.	yes
La	C23	2.637(4)	.	.	yes
La	C15	2.779(4)	.	3_555	yes
N1	C1	1.470(6)	.	.	yes
N1	C2	1.472(6)	.	.	yes
N1	C8	1.483(6)	.	.	yes
N2	C3	1.490(6)	.	.	yes
N2	C4	1.490(6)	.	.	yes
N2	C5	1.490(6)	.	.	yes
N3	C6	1.470(5)	.	.	yes
N3	C9	1.448(5)	.	.	yes
N4	C10	1.467(6)	.	.	yes
N4	C11	1.484(5)	.	.	yes
N4	C14	1.499(6)	.	.	yes
C2	C3	1.525(6)	.	.	no
C5	C6	1.525(6)	.	.	no
C6	C7	1.532(6)	.	.	no
C6	C8	1.542(6)	.	.	no
C9	C10	1.521(6)	.	.	no
C11	C12	1.519(6)	.	.	no
C12	C13	1.541(6)	.	.	no
C13	C14	1.535(6)	.	.	no
C15	C16	1.225(6)	.	.	no
C16	C17	1.438(6)	.	.	no
C17	C18	1.381(6)	.	.	no
C17	C22	1.400(6)	.	.	no
C18	C19	1.384(6)	.	.	no
C19	C20	1.386(6)	.	.	no
C20	C21	1.379(6)	.	.	no
C21	C22	1.387(6)	.	.	no
C23	C24	1.219(6)	.	.	no
C24	C25	1.435(6)	.	.	no
C25	C26	1.401(6)	.	.	no
C25	C30	1.394(7)	.	.	no
C26	C27	1.374(6)	.	.	no
C27	C28	1.374(8)	.	.	no
C28	C29	1.383(8)	.	.	no
C29	C30	1.389(8)	.	.	no
C1	H1	0.9800	.	.	no
C1	H1'	0.9800	.	.	no
C1	H1''	0.9800	.	.	no
C2	H2	0.9900	.	.	no
C2	H2'	0.9900	.	.	no
C3	H3	0.9900	.	.	no
C3	H3'	0.9900	.	.	no
C4	H4	0.9800	.	.	no
C4	H4'	0.9800	.	.	no
C4	H4''	0.9800	.	.	no
C5	H5	0.9900	.	.	no
C5	H5'	0.9900	.	.	no
C7	H7	0.9800	.	.	no
C7	H7'	0.9800	.	.	no
C7	H7''	0.9800	.	.	no
C8	H8	0.9900	.	.	no
C8	H8'	0.9900	.	.	no
C9	H9	0.9900	.	.	no
C9	H9'	0.9900	.	.	no
C10	H10	0.9900	.	.	no
C10	H10'	0.9900	.	.	no
C11	H11	0.9900	.	.	no
C11	H11'	0.9900	.	.	no

C12	H12	0.9900	.	.	no
C12	H12'	0.9900	.	.	no
C13	H13	0.9900	.	.	no
C13	H13'	0.9900	.	.	no
C14	H14	0.9900	.	.	no
C14	H14'	0.9900	.	.	no
C18	H18	0.9500	.	.	no
C19	H19	0.9500	.	.	no
C20	H20	0.9500	.	.	no
C21	H21	0.9500	.	.	no
C22	H22	0.9500	.	.	no
C26	H26	0.9500	.	.	no
C27	H27	0.9500	.	.	no
C28	H28	0.9500	.	.	no
C29	H29	0.9500	.	.	no
C30	H30	0.9500	.	.	no
loop_					
_geom_angle_atom_site_label_1					
_geom_angle_atom_site_label_2					
_geom_angle_atom_site_label_3					
_geom_angle					
_geom_angle_site_symmetry_1					
_geom_angle_site_symmetry_2					
_geom_angle_site_symmetry_3					
_geom_angle_publ_flag					
N1	La	N2	59.38(11)	.	yes
N1	La	N3	65.69(12)	.	yes
N1	La	N4	115.49(12)	.	yes
N1	La	C15	85.47(11)	.	yes
N1	La	C23	153.28(11)	.	yes
N1	La	C15	81.62(12)	3_555	yes
N2	La	N3	69.80(12)	.	yes
N2	La	N4	131.48(12)	.	yes
N2	La	C15	139.39(13)	.	yes
N2	La	C23	94.14(13)	.	yes
N2	La	C15	79.36(13)	3_555	yes
N3	La	N4	65.98(10)	.	yes
N3	La	C15	116.01(13)	.	yes
N3	La	C23	110.96(13)	.	yes
N3	La	C15	143.16(11)	3_555	yes
N4	La	C15	79.85(12)	.	yes
N4	La	C23	83.93(13)	.	yes
N4	La	C15	148.88(11)	3_555	yes
C15	La	C23	117.35(13)	.	yes
C15	La	C15	75.69(13)	3_555	yes
C15	La	C23	90.43(13)	3_555	yes
La	N1	C1	115.2(2)	.	yes
La	N1	C2	106.1(3)	.	yes
La	N1	C8	106.9(3)	.	yes
C1	N1	C2	108.2(4)	.	yes
C1	N1	C8	109.1(3)	.	yes
C2	N1	C8	111.5(3)	.	yes
La	N2	C3	112.9(2)	.	yes
La	N2	C4	113.7(2)	.	yes
La	N2	C5	104.5(2)	.	yes
C3	N2	C4	107.6(3)	.	yes
C3	N2	C5	109.9(3)	.	yes
C4	N2	C5	108.1(3)	.	yes
La	N3	C6	115.7(2)	.	yes
La	N3	C9	122.5(2)	.	yes

C6	N3	C9	115.9(3)	.	.	.	yes
La	N4	C10	97.0(2)	.	.	.	yes
La	N4	C11	118.6(3)	.	.	.	yes
La	N4	C14	114.8(2)	.	.	.	yes
C10	N4	C11	112.0(3)	.	.	.	yes
C10	N4	C14	110.9(4)	.	.	.	yes
C11	N4	C14	103.7(3)	.	.	.	yes
N1	C2	C3	114.4(4)	.	.	.	yes
N2	C3	C2	114.4(3)	.	.	.	yes
N2	C5	C6	114.0(3)	.	.	.	yes
N3	C6	C5	107.7(3)	.	.	.	yes
N3	C6	C7	115.2(3)	.	.	.	yes
N3	C6	C8	107.8(3)	.	.	.	yes
C5	C6	C7	106.4(3)	.	.	.	no
C5	C6	C8	111.2(3)	.	.	.	no
C7	C6	C8	108.6(3)	.	.	.	no
N1	C8	C6	112.5(3)	.	.	.	yes
N3	C9	C10	111.1(3)	.	.	.	yes
N4	C10	C9	112.0(3)	.	.	.	yes
N4	C11	C12	103.5(3)	.	.	.	yes
C11	C12	C13	103.7(3)	.	.	.	no
C12	C13	C14	105.7(3)	.	.	.	no
N4	C14	C13	104.9(3)	.	.	.	yes
La	C15	C16	134.7(3)	.	.	.	yes
La	C15	La	104.31(14)	.	.	3_555	yes
La	C15	C16	112.8(3)	3_555	.	.	yes
C15	C16	C17	179.2(4)	.	.	.	no
C16	C17	C18	121.4(4)	.	.	.	no
C16	C17	C22	120.2(4)	.	.	.	no
C18	C17	C22	118.4(4)	.	.	.	no
C17	C18	C19	121.4(4)	.	.	.	no
C18	C19	C20	119.7(4)	.	.	.	no
C19	C20	C21	119.9(4)	.	.	.	no
C20	C21	C22	120.2(4)	.	.	.	no
C17	C22	C21	120.4(4)	.	.	.	no
La	C23	C24	172.0(4)	.	.	.	yes
C23	C24	C25	176.3(5)	.	.	.	no
C24	C25	C26	120.5(4)	.	.	.	no
C24	C25	C30	122.1(4)	.	.	.	no
C26	C25	C30	117.4(4)	.	.	.	no
C25	C26	C27	121.5(4)	.	.	.	no
C26	C27	C28	120.3(5)	.	.	.	no
C27	C28	C29	119.7(5)	.	.	.	no
C28	C29	C30	120.3(5)	.	.	.	no
C25	C30	C29	120.8(5)	.	.	.	no
N1	C1	H1	109.00	.	.	.	no
N1	C1	H1'	109.00	.	.	.	no
N1	C1	H1''	109.00	.	.	.	no
H1	C1	H1'	109.00	.	.	.	no
H1	C1	H1''	109.00	.	.	.	no
H1'	C1	H1''	110.00	.	.	.	no
N1	C2	H2	109.00	.	.	.	no
N1	C2	H2'	109.00	.	.	.	no
C3	C2	H2	109.00	.	.	.	no
C3	C2	H2'	109.00	.	.	.	no
H2	C2	H2'	108.00	.	.	.	no
N2	C3	H3	109.00	.	.	.	no
N2	C3	H3'	109.00	.	.	.	no
C2	C3	H3	109.00	.	.	.	no
C2	C3	H3'	109.00	.	.	.	no
H3	C3	H3'	108.00	.	.	.	no

N2	C4	H4	109.00	.	.	.	no
N2	C4	H4'	110.00	.	.	.	no
N2	C4	H4"	109.00	.	.	.	no
H4	C4	H4'	110.00	.	.	.	no
H4	C4	H4"	109.00	.	.	.	no
H4'	C4	H4"	109.00	.	.	.	no
N2	C5	H5	109.00	.	.	.	no
N2	C5	H5'	109.00	.	.	.	no
C6	C5	H5	109.00	.	.	.	no
C6	C5	H5'	109.00	.	.	.	no
H5	C5	H5'	108.00	.	.	.	no
C6	C7	H7	109.00	.	.	.	no
C6	C7	H7'	110.00	.	.	.	no
C6	C7	H7"	109.00	.	.	.	no
H7	C7	H7'	109.00	.	.	.	no
H7	C7	H7"	109.00	.	.	.	no
H7'	C7	H7"	109.00	.	.	.	no
N1	C8	H8	109.00	.	.	.	no
N1	C8	H8'	109.00	.	.	.	no
C6	C8	H8	109.00	.	.	.	no
C6	C8	H8'	109.00	.	.	.	no
H8	C8	H8'	108.00	.	.	.	no
N3	C9	H9	109.00	.	.	.	no
N3	C9	H9'	109.00	.	.	.	no
C10	C9	H9	109.00	.	.	.	no
C10	C9	H9'	109.00	.	.	.	no
H9	C9	H9'	108.00	.	.	.	no
N4	C10	H10	109.00	.	.	.	no
N4	C10	H10'	109.00	.	.	.	no
C9	C10	H10	109.00	.	.	.	no
C9	C10	H10'	109.00	.	.	.	no
H10	C10	H10'	108.00	.	.	.	no
N4	C11	H11	111.00	.	.	.	no
N4	C11	H11'	111.00	.	.	.	no
C12	C11	H11	111.00	.	.	.	no
C12	C11	H11'	111.00	.	.	.	no
H11	C11	H11'	109.00	.	.	.	no
C11	C12	H12	111.00	.	.	.	no
C11	C12	H12'	111.00	.	.	.	no
C13	C12	H12	111.00	.	.	.	no
C13	C12	H12'	111.00	.	.	.	no
H12	C12	H12'	109.00	.	.	.	no
C12	C13	H13	111.00	.	.	.	no
C12	C13	H13'	111.00	.	.	.	no
C14	C13	H13	111.00	.	.	.	no
C14	C13	H13'	111.00	.	.	.	no
H13	C13	H13'	109.00	.	.	.	no
N4	C14	H14	111.00	.	.	.	no
N4	C14	H14'	111.00	.	.	.	no
C13	C14	H14	111.00	.	.	.	no
C13	C14	H14'	111.00	.	.	.	no
H14	C14	H14'	109.00	.	.	.	no
C17	C18	H18	119.00	.	.	.	no
C19	C18	H18	119.00	.	.	.	no
C18	C19	H19	120.00	.	.	.	no
C20	C19	H19	120.00	.	.	.	no
C19	C20	H20	120.00	.	.	.	no
C21	C20	H20	120.00	.	.	.	no
C20	C21	H21	120.00	.	.	.	no
C22	C21	H21	120.00	.	.	.	no
C17	C22	H22	120.00	.	.	.	no

C21	C22	H22	120.00	.	.	.	no
C25	C26	H26	119.00	.	.	.	no
C27	C26	H26	119.00	.	.	.	no
C26	C27	H27	120.00	.	.	.	no
C28	C27	H27	120.00	.	.	.	no
C27	C28	H28	120.00	.	.	.	no
C29	C28	H28	120.00	.	.	.	no
C28	C29	H29	120.00	.	.	.	no
C30	C29	H29	120.00	.	.	.	no
C25	C30	H30	120.00	.	.	.	no
C29	C30	H30	120.00	.	.	.	no

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

N2	La	N1	C1	-166.1(3)	.	.	.	.	no
N2	La	N1	C2	-46.4(2)	.	.	.	.	no
N2	La	N1	C8	72.6(2)	.	.	.	.	no
N3	La	N1	C1	113.9(3)	.	.	.	.	no
N3	La	N1	C2	-126.5(3)	.	.	.	.	no
N3	La	N1	C8	-7.5(2)	.	.	.	.	no
N4	La	N1	C1	69.2(3)	.	.	.	.	no
N4	La	N1	C2	-171.2(2)	.	.	.	.	no
N4	La	N1	C8	-52.2(3)	.	.	.	.	no
C15	La	N1	C1	-7.3(3)	.	.	.	.	no
C15	La	N1	C2	112.3(3)	.	.	.	.	no
C15	La	N1	C8	-128.7(3)	.	.	.	.	no
C23	La	N1	C1	-157.5(3)	.	.	.	.	no
C23	La	N1	C2	-37.9(4)	.	.	.	.	no
C23	La	N1	C8	81.2(4)	.	.	.	.	no
C15	La	N1	C1	-83.5(3)	3_555	.	.	.	no
C15	La	N1	C2	36.1(3)	3_555	.	.	.	no
C15	La	N1	C8	155.1(3)	3_555	.	.	.	no
N1	La	N2	C3	41.9(3)	.	.	.	.	no
N1	La	N2	C4	164.9(3)	.	.	.	.	no
N1	La	N2	C5	-77.5(3)	.	.	.	.	no
N3	La	N2	C3	115.0(3)	.	.	.	.	no
N3	La	N2	C4	-122.1(3)	.	.	.	.	no
N3	La	N2	C5	-4.5(2)	.	.	.	.	no
N4	La	N2	C3	140.2(3)	.	.	.	.	no
N4	La	N2	C4	-96.8(3)	.	.	.	.	no
N4	La	N2	C5	20.8(3)	.	.	.	.	no
C15	La	N2	C3	8.2(4)	.	.	.	.	no
C15	La	N2	C4	131.2(3)	.	.	.	.	no
C15	La	N2	C5	-111.3(3)	.	.	.	.	no
C23	La	N2	C3	-134.2(3)	.	.	.	.	no
C23	La	N2	C4	-11.2(3)	.	.	.	.	no
C23	La	N2	C5	106.3(3)	.	.	.	.	no
C15	La	N2	C3	-44.6(3)	3_555	.	.	.	no
C15	La	N2	C4	78.4(3)	3_555	.	.	.	no
C15	La	N2	C5	-164.0(3)	3_555	.	.	.	no
N1	La	N3	C6	37.9(3)	.	.	.	.	no
N1	La	N3	C9	-113.8(3)	.	.	.	.	no

N2	La	N3	C6	-26.7(3)	.	.	.	.	no
N2	La	N3	C9	-178.4(3)	.	.	.	.	no
N4	La	N3	C6	173.8(3)	.	.	.	.	no
N4	La	N3	C9	22.1(3)	.	.	.	.	no
C15	La	N3	C6	109.4(3)	.	.	.	.	no
C15	La	N3	C9	-42.3(3)	.	.	.	.	no
C23	La	N3	C6	-113.3(3)	.	.	.	.	no
C23	La	N3	C9	95.0(3)	.	.	.	.	no
C15	La	N3	C6	8.3(4)	3_555	.	.	.	no
C15	La	N3	C9	-143.4(3)	3_555	.	.	.	no
N1	La	N4	C10	3.9(3)	.	.	.	.	no
N1	La	N4	C11	-115.9(3)	.	.	.	.	no
N1	La	N4	C14	120.8(3)	.	.	.	.	no
N2	La	N4	C10	-66.7(3)	.	.	.	.	no
N2	La	N4	C11	173.5(3)	.	.	.	.	no
N2	La	N4	C14	50.2(3)	.	.	.	.	no
N3	La	N4	C10	-40.7(2)	.	.	.	.	no
N3	La	N4	C11	-160.5(3)	.	.	.	.	no
N3	La	N4	C14	76.2(3)	.	.	.	.	no
C15	La	N4	C10	83.9(2)	.	.	.	.	no
C15	La	N4	C11	-35.9(3)	.	.	.	.	no
C15	La	N4	C14	-159.2(3)	.	.	.	.	no
C23	La	N4	C10	-156.9(3)	.	.	.	.	no
C23	La	N4	C11	83.3(3)	.	.	.	.	no
C23	La	N4	C14	-40.0(3)	.	.	.	.	no
C15	La	N4	C10	122.4(3)	3_555	.	.	.	no
C15	La	N4	C11	2.6(4)	3_555	.	.	.	no
C15	La	N4	C14	-120.7(3)	3_555	.	.	.	no
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N1	La	C15	La	-82.49(14)	.	.	.	3_555	no
N2	La	C15	C16	90.8(5)	.	.	.	.	no
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N3	La	C15	C16	2.0(5)	.	.	.	.	no
N3	La	C15	La	-142.61(12)	.	.	.	3_555	no
N4	La	C15	C16	-54.8(5)	.	.	.	.	no
N4	La	C15	La	160.59(15)	.	.	.	3_555	no
C23	La	C15	C16	-132.5(5)	.	.	.	.	no
C23	La	C15	La	82.92(17)	.	.	.	3_555	no
C15	La	C15	C16	144.6(5)	3_555	.	.	.	no
C15	La	C15	La	0.00(13)	3_555	.	.	3_555	no
N1	La	C15	La	87.43(13)	.	.	3_555	3_555	no
N1	La	C15	C16	-119.1(3)	.	.	3_555	3_555	no
N2	La	C15	La	147.69(16)	.	.	3_555	3_555	no
N2	La	C15	C16	-58.9(3)	.	.	3_555	3_555	no
N3	La	C15	La	114.5(2)	.	.	3_555	3_555	no
N3	La	C15	C16	-92.1(4)	.	.	3_555	3_555	no
N4	La	C15	La	-39.3(3)	.	.	3_555	3_555	no
N4	La	C15	C16	114.2(4)	.	.	3_555	3_555	no
C15	La	C15	La	0.00(13)	.	.	3_555	3_555	no
C15	La	C15	C16	153.5(4)	.	.	3_555	3_555	no
C23	La	C15	La	-118.18(15)	.	.	3_555	3_555	no
C23	La	C15	C16	35.3(3)	.	.	3_555	3_555	no
La	N1	C2	C3	49.5(4)	.	.	.	.	no
C1	N1	C2	C3	173.6(3)	.	.	.	.	no
C8	N1	C2	C3	-66.5(5)	.	.	.	.	no
La	N1	C8	C6	-21.0(4)	.	.	.	.	no
C1	N1	C8	C6	-146.2(3)	.	.	.	.	no
C2	N1	C8	C6	94.4(4)	.	.	.	.	no
La	N2	C3	C2	-34.1(4)	.	.	.	.	no
C4	N2	C3	C2	-160.4(3)	.	.	.	.	no
C5	N2	C3	C2	82.1(4)	.	.	.	.	no

La	N2	C5	C6	34.0(4)	.	.	.	.	no
C3	N2	C5	C6	-87.5(4)	.	.	.	.	no
C4	N2	C5	C6	155.4(3)	.	.	.	.	no
La	N3	C6	C5	54.6(4)	.	.	.	.	no
La	N3	C6	C7	173.2(3)	.	.	.	.	no
La	N3	C6	C8	-65.5(4)	.	.	.	.	no
C9	N3	C6	C5	-151.7(3)	.	.	.	.	no
C9	N3	C6	C7	-33.2(5)	.	.	.	.	no
C9	N3	C6	C8	88.2(4)	.	.	.	.	no
La	N3	C9	C10	1.3(5)	.	.	.	.	no
C6	N3	C9	C10	-150.4(3)	.	.	.	.	no
La	N4	C10	C9	58.8(3)	.	.	.	.	no
C11	N4	C10	C9	-176.5(4)	.	.	.	.	no
C14	N4	C10	C9	-61.2(4)	.	.	.	.	no
La	N4	C11	C12	-84.7(3)	.	.	.	.	no
C10	N4	C11	C12	163.6(4)	.	.	.	.	no
C14	N4	C11	C12	44.0(4)	.	.	.	.	no
La	N4	C14	C13	96.6(3)	.	.	.	.	no
C10	N4	C14	C13	-154.7(3)	.	.	.	.	no
C11	N4	C14	C13	-34.3(4)	.	.	.	.	no
N1	C2	C3	N2	-12.8(5)	.	.	.	.	no
N2	C5	C6	N3	-59.3(4)	.	.	.	.	no
N2	C5	C6	C7	176.7(3)	.	.	.	.	no
N2	C5	C6	C8	58.7(5)	.	.	.	.	no
N3	C6	C8	N1	53.5(4)	.	.	.	.	no
C5	C6	C8	N1	-64.4(4)	.	.	.	.	no
C7	C6	C8	N1	178.9(3)	.	.	.	.	no
N3	C9	C10	N4	-47.7(5)	.	.	.	.	no
N4	C11	C12	C13	-35.9(4)	.	.	.	.	no
C11	C12	C13	C14	14.5(4)	.	.	.	.	no
C12	C13	C14	N4	11.7(4)	.	.	.	.	no
C16	C17	C18	C19	-178.4(4)	.	.	.	.	no
C22	C17	C18	C19	0.1(6)	.	.	.	.	no
C16	C17	C22	C21	177.7(4)	.	.	.	.	no
C18	C17	C22	C21	-0.8(6)	.	.	.	.	no
C17	C18	C19	C20	0.1(7)	.	.	.	.	no
C18	C19	C20	C21	0.3(6)	.	.	.	.	no
C19	C20	C21	C22	-1.0(6)	.	.	.	.	no
C20	C21	C22	C17	1.3(6)	.	.	.	.	no
C24	C25	C26	C27	-178.7(4)	.	.	.	.	no
C30	C25	C26	C27	0.5(6)	.	.	.	.	no
C24	C25	C30	C29	178.2(4)	.	.	.	.	no
C26	C25	C30	C29	-1.0(6)	.	.	.	.	no
C25	C26	C27	C28	0.1(7)	.	.	.	.	no
C26	C27	C28	C29	-0.1(7)	.	.	.	.	no
C27	C28	C29	C30	-0.3(7)	.	.	.	.	no
C28	C29	C30	C25	0.9(7)	.	.	.	.	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

La	C1	4.498(4)	.	3_555	no
La	C21	4.496(4)	.	4_555	no
La	H12'	3.8500	.	.	no
La	H1'	3.6400	.	3_555	no
La	H2	4.0700	.	3_555	no
La	H21	3.7200	.	4_555	no

N1	N2	2.766(6)	.	.	no
N1	N3	2.847(5)	.	.	no
N1	C3	2.519(6)	.	.	no
N1	C5	3.048(6)	.	.	no
N1	C6	2.515(6)	.	.	no
N2	N1	2.766(6)	.	.	no
N2	N3	2.918(5)	.	.	no
N2	C2	2.535(6)	.	.	no
N2	C6	2.528(6)	.	.	no
N2	C8	3.018(6)	.	.	no
N3	N1	2.847(5)	.	.	no
N3	N2	2.918(5)	.	.	no
N3	N4	2.812(4)	.	.	no
N3	C5	2.419(5)	.	.	no
N3	C8	2.434(5)	.	.	no
N3	C10	2.448(5)	.	.	no
N3	C14	3.327(5)	.	.	no
N4	N3	2.812(4)	.	.	no
N4	C9	2.476(5)	.	.	no
N3	H14	2.9400	.	.	no
C1	C16	3.584(6)	.	.	no
C1	La	4.498(4)	.	3_555	no
C3	C16	3.570(6)	.	3_555	no
C4	C16	3.564(6)	.	3_555	no
C13	C23	3.477(6)	.	.	no
C15	C11	3.490(6)	.	.	no
C15	C2	3.378(6)	.	3_555	no
C15	C3	3.439(6)	.	3_555	no
C15	C1	3.534(6)	.	.	no
C15	C15	3.344(6)	.	3_555	no
C16	C4	3.564(6)	.	3_555	no
C16	C3	3.570(6)	.	3_555	no
C16	C1	3.584(6)	.	.	no
C18	C26	3.534(6)	.	3_555	no
C18	C24	3.511(6)	.	3_555	no
C21	C23	3.552(6)	.	4_454	no
C21	La	4.496(4)	.	4_454	no
C23	C21	3.552(6)	.	4_555	no
C23	C13	3.477(6)	.	.	no
C24	C18	3.511(6)	.	3_555	no
C26	C18	3.534(6)	.	3_555	no
C3	H8	2.9800	.	.	no
C7	H9'	2.6100	.	.	no
C7	H1	3.0900	.	2_455	no
C7	H9	2.9200	.	.	no
C8	H9'	2.9300	.	.	no
C9	H7"	2.6300	.	.	no
C9	H28	3.0900	.	1_455	no
C9	H14	2.8600	.	.	no
C9	H8'	3.0100	.	.	no
C9	H14'	2.9700	.	.	no
C9	H7	2.9600	.	.	no
C13	H8	3.0600	.	4_554	no
C14	H9	2.7200	.	.	no
C15	H11'	2.7200	.	.	no
C15	H2	2.7900	.	3_555	no
C15	H3'	3.0600	.	3_555	no
C16	H4"	2.7900	.	3_555	no
C16	H1"	3.0400	.	.	no
C16	H3'	2.9400	.	3_555	no
C16	H10	2.9600	.	.	no

C16	H11'	2.7900	.	.	no
C17	H4"	2.6500	.	3_555	no
C18	H4"	2.9800	.	3_555	no
C18	H27	2.9700	.	1_455	no
C19	H11	3.0100	.	2_444	no
C20	H14'	2.9700	.	2_444	no
C20	H5	2.8000	.	4_454	no
C20	H14	3.0600	.	4_454	no
C21	H4'	2.8300	.	4_454	no
C21	H14	2.9200	.	4_454	no
C21	H5	2.9200	.	4_454	no
C22	H4'	2.9800	.	4_454	no
C23	H18	2.9000	.	3_555	no
C23	H1'	2.8800	.	3_555	no
C23	H13	2.8600	.	.	no
C23	H21	2.6700	.	4_555	no
C24	H13	3.0000	.	.	no
C24	H7'	3.0400	.	4_554	no
C24	H21	3.0400	.	4_555	no
C24	H18	2.6400	.	3_555	no
C25	H5'	3.0400	.	4_554	no
C25	H7'	3.0400	.	4_554	no
C25	H18	2.9300	.	3_555	no
C26	H18	2.7900	.	3_555	no
C26	H5'	3.0400	.	4_554	no
C26	H7'	3.0300	.	4_554	no
C28	H4	2.9800	.	4_554	no
C30	H5'	3.0800	.	4_554	no
H1	H2'	2.4400	.	.	no
H1	H8'	2.4600	.	.	no
H1	C7	3.0900	.	2_445	no
H1'	H2	2.2500	.	.	no
H1'	La	3.6400	.	3_555	no
H1'	C23	2.8800	.	3_555	no
H1"	C16	3.0400	.	.	no
H1"	H8'	2.2800	.	.	no
H2	H1'	2.2500	.	.	no
H2	La	4.0700	.	3_555	no
H2	C15	2.7900	.	3_555	no
H2'	H1	2.4400	.	.	no
H2'	H8	2.2400	.	.	no
H3	H4	2.5500	.	.	no
H3	H5'	2.1000	.	.	no
H3'	H4"	2.2300	.	.	no
H3'	C15	3.0600	.	3_555	no
H3'	C16	2.9400	.	3_555	no
H4	H3	2.5500	.	.	no
H4	H5	2.5600	.	.	no
H4	C28	2.9800	.	4_455	no
H4'	H5	2.2600	.	.	no
H4'	C21	2.8300	.	4_555	no
H4'	C22	2.9800	.	4_555	no
H4"	H3'	2.2300	.	.	no
H4"	C16	2.7900	.	3_555	no
H4"	C17	2.6500	.	3_555	no
H4"	C18	2.9800	.	3_555	no
H5	H4	2.5600	.	.	no
H5	H4'	2.2600	.	.	no
H5	H7	2.4400	.	.	no
H5	C20	2.8000	.	4_555	no
H5	C21	2.9200	.	4_555	no

H5'	H3	2.1000	.	.	no
H5'	H7'	2.3500	.	.	no
H5'	H8	2.5300	.	.	no
H5'	C25	3.0400	.	4_455	no
H5'	C26	3.0400	.	4_455	no
H5'	C30	3.0800	.	4_455	no
H7	C9	2.9600	.	.	no
H7	H5	2.4400	.	.	no
H7	H20	2.5700	.	4_555	no
H7'	H5'	2.3500	.	.	no
H7'	H8	2.5000	.	.	no
H7'	C24	3.0400	.	4_455	no
H7'	C25	3.0400	.	4_455	no
H7'	C26	3.0300	.	4_455	no
H7"	C9	2.6300	.	.	no
H7"	H8'	2.4400	.	.	no
H7"	H9'	2.0800	.	.	no
H8	C3	2.9800	.	.	no
H8	H2'	2.2400	.	.	no
H8	H5'	2.5300	.	.	no
H8	H7'	2.5000	.	.	no
H8	C13	3.0600	.	4_455	no
H8'	C9	3.0100	.	.	no
H8'	H1	2.4600	.	.	no
H8'	H1"	2.2800	.	.	no
H8'	H7"	2.4400	.	.	no
H8'	H9'	2.4600	.	.	no
H8'	H12	2.5900	.	4_455	no
H9	C7	2.9200	.	.	no
H9	C14	2.7200	.	.	no
H9	H14	2.5200	.	.	no
H9	H14'	2.5400	.	.	no
H9	H20	2.5900	.	4_555	no
H9'	C7	2.6100	.	.	no
H9'	C8	2.9300	.	.	no
H9'	H7"	2.0800	.	.	no
H9'	H8'	2.4600	.	.	no
H9'	H28	2.2700	.	1_455	no
H10	C16	2.9600	.	.	no
H10'	H11	2.3500	.	.	no
H10'	H14'	2.3400	.	.	no
H11	H10'	2.3500	.	.	no
H11	C19	3.0100	.	2_454	no
H11'	C15	2.7200	.	.	no
H11'	C16	2.7900	.	.	no
H11'	H22	2.5300	.	.	no
H12	H8'	2.5900	.	4_554	no
H12'	La	3.8500	.	.	no
H13	C23	2.8600	.	.	no
H13	C24	3.0000	.	.	no
H14	N3	2.9400	.	.	no
H14	C9	2.8600	.	.	no
H14	H9	2.5200	.	.	no
H14	C20	3.0600	.	4_555	no
H14	C21	2.9200	.	4_555	no
H14	H20	2.6000	.	4_555	no
H14	H21	2.2900	.	4_555	no
H14'	C9	2.9700	.	.	no
H14'	H9	2.5400	.	.	no
H14'	H10'	2.3400	.	.	no
H14'	C20	2.9700	.	2_454	no

H14'	H20	2.5600	.	2_454	no
H18	C23	2.9000	.	3_555	no
H18	C24	2.6400	.	3_555	no
H18	C25	2.9300	.	3_555	no
H18	C26	2.7900	.	3_555	no
H18	H26	2.3900	.	3_555	no
H20	H14'	2.5600	.	2_444	no
H20	H7	2.5700	.	4_454	no
H20	H9	2.5900	.	4_454	no
H20	H14	2.6000	.	4_454	no
H21	La	3.7200	.	4_454	no
H21	C23	2.6700	.	4_454	no
H21	C24	3.0400	.	4_454	no
H21	H14	2.2900	.	4_454	no
H22	H11'	2.5300	.	.	no
H22	H30	2.5200	.	4_454	no
H26	H18	2.3900	.	3_555	no
H27	C18	2.9700	.	1_655	no
H28	C9	3.0900	.	1_655	no
H28	H9'	2.2700	.	1_655	no
H30	H22	2.5200	.	4_555	no

#===END of Crystallographic Information File