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Synthesis and structural characterisation of a boralumoxane capable of activating a zirconocene ethene polymerisation catalyst

Richter, B.; Meetsma, A.; Hessen, B.; Teuben, J.H

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1. SUBMISSION DETAILS

_publ_contact_author_name # Name of author for correspondence
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Dr. B. Hessen
;
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_publ_requested_category ?
_publ_requested_coeditor_name ?

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Date of submission : 2001-05-23
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boraluminoxane capable of activating a zirconocene
ethene polymerisation catalyst

to be submitted to : Chemical Communications

Your Reference number : B103670J
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_year                  ?
_journal_volume                ?
_journal_issue                 ?
_journal_page_first           ?
_journal_page_last            ?

_journal_suppl_publ_number     ?
_journal_suppl_publ_pages      ?

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# 3. TITLE AND AUTHOR LIST

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The reaction of But-Al with ArB(OH)-2
(Ar=2,6-diisopropylphenyl) leads, via the
intermediate [But-Al(O)BAr(OH)]-2 (1), to the
crystallographically characterised boraluminoxane
Al(But-Al)(ButAl)-2-(O-2-BAr)-4 (3)
which is able to activate Cp-2-ZrMe-2 to effect
catalytic ethene polymerisation.

;
_publ_section_title_footnote
;
?
;

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

loop_
_publ_author_name
_publ_author_address

'Richter, Bodo'
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Dutch Polymer Institute
Centre for Catalytic Olefin Polymerisation,
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;
'Meetsma, Auke'
;
Dutch Polymer Institute
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```

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'Hessen, Bart'
;

Dutch Polymer Institute
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;
'Teuben, Jan H.'
;

Dutch Polymer Institute
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Nijenborgh 4,
NL-9747 AG Groningen,
The Netherlands.

;

#=====

4. TEXT

_publ_section_synopsis

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_publ_section_exptl_refinement

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;

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;

Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\`ia-Granda, S.
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;

_publ_section_figure_captions

;

Fig. 1. Chemical structural diagram (scheme 1) of the title compound

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

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

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

;

=====

#data_c79h119a

=====

5. CHEMICAL DATA

_chemical_name_systematic

;

?

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety

'C64 H104 Al4 B4 O8, 2.5(C6 H6)'

```

_chemical_formula_structural      ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C79 H119 Al4 B4 O8'
_chemical_formula_weight          1347.96
_chemical_compound_source         'see text'

```

```

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_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
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O   O   0.0106   0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
B   B   0.0013   0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Al  Al   0.0645   0.0514
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H   H   0.0000   0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C   C   0.0033   0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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```

#=====

```

6. CRYSTAL DATA

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_symmetry_space_group_name_H-M    'P -1'

```

```

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

```

```

_cell_length_a                    14.0027(5)
_cell_length_b                    14.2483(5)
_cell_length_c                    22.7478(9)
_cell_angle_alpha                 79.888(1)
_cell_angle_beta                 86.886(1)
_cell_angle_gamma                 65.389(1)
_cell_volume                      4061.2(3)
_cell_formula_units_Z             2
_cell_measurement_temperature     200
_cell_measurement_reflns_used     9078
_cell_measurement_theta_min       2.33
_cell_measurement_theta_max       28.29
_cell_special_details
;

```

The final unit cell was obtained from the xyz centroids of 9078 reflections after integration using the SAINT software package (Bruker, 2000).
Intensity data were corrected for decay and absorption using SADABS (Sheldrick, 2000)

```

_exptl_crystal_description        'block'
_exptl_crystal_colour             'colorless'
_exptl_crystal_size_max           0.500
_exptl_crystal_size_mid           0.480
_exptl_crystal_size_min           0.120

```

```

_exptl_crystal_size_rad      ?
_exptl_crystal_density_meas  ?
_exptl_crystal_density_diffn 1.102
_exptl_crystal_density_method 'Not Measured'
_exptl_crystal_F_000         1458
_exptl_absorpt_coefficient_mu 0.108
_exptl_absorpt_correction_type 'Multi-Scan'
_exptl_absorpt_process_details 'Sheldrick, Bruker, 2000)'
_exptl_absorpt_correction_T_min 0.9482
_exptl_absorpt_correction_T_max 0.9872

```

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

``` # 7. EXPERIMENTAL DATA ```

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?
;

_diffn_ambient_temperature 200(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
;
_diffn_measurement_method    'phi and omega scans'

_diffn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature
unit (KRYOFLEX, (Bruker, 2000)).
;
_diffn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'

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_diffn_standards_interval_count ?
_diffn_standards_interval_time ?
_diffn_standards_decay_%     ?

loop_
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_diffn_standard_refl_index_k
_diffn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffn_refl_number          38591
_diffn_refl_av_R_equivalents 0.0274
_diffn_refl_av_sigmaI/netI  0.0559
_diffn_refl_limit_h_min     -19
_diffn_refl_limit_h_max     18
_diffn_refl_limit_k_min     -18
_diffn_refl_limit_k_max     19
_diffn_refl_limit_l_min     -29
_diffn_refl_limit_l_max     30

```

```
_diffrn_reflns_theta_min      2.33
_diffrn_reflns_theta_max      29.02
_diffrn_measured_fraction_theta_max  0.944
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_diffrn_measured_fraction_theta_full  0.944
```

```
_diffrn_reflns_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)

Intensity data were corrected for Lorentz and polarization effects, scale variation, for absorption and reduced to F_o^2

```
;
```

```
# number of unique reflections
```

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_reflns_number_total      20435
_reflns_number_gt         13923
_reflns_threshold_expression >2sigma(I)
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_computing_cell_refinement      'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction      'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
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```
;
```

```
DIRDIF-99 (Beurskens et al., 1999)
```

```
;
```

```
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
```

```
;
```

```
PLUTO (Meetsma, 2001)
```

```
PLATON (Spek, 1994)
```

```
;
```

```
_computing_publication_material
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```
;
```

```
PLATON (Spek, 1990)
```

```
SHELXL (Sheldrick, 1997)
```

```
;
```

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

8. REFINEMENT DATA

```
_refine_special_details
```

```
;
```

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program DIRDIF.

The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined.

Refinement was frustrated by a disorder problem: from the solution it was clear that one of the benzene solvent molecules was highly disordered.

The electron density of the carbon atoms appeared to be spread out, indicating transformational disorder. This molecule was fitted to two partial occupied regular hexagons (with consequence of large a.d.p.s)

The hydrogen atoms were included in the final refinement riding on their carrier atoms.

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/[\s^2^(Fo^2^)+(0.0889P)^2^+0.5086P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     Patterson
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   difmap
_refine_ls_hydrogen_treatment    refall
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_refine_ls_number_reflns         20435
_refine_ls_number_parameters      912
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_refine_ls_R_factor_gt           0.0582
_refine_ls_wR_factor_ref         0.1689
_refine_ls_wR_factor_gt          0.1498
_refine_ls_goodness_of_fit_ref    1.030
_refine_ls_restrained_S_all       1.030
_refine_ls_shift/su_max           0.618
_refine_ls_shift/su_mean          0.044

_refine_diff_density_max          0.686
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_refine_diff_density_rms          0.056
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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
Al1 Al Uani 0.30442(4) 0.95613(4) 0.27023(2) 1.000 0.0212(2) . .
Al2 Al Uani 0.56154(4) 0.83274(4) 0.31351(3) 1.000 0.0282(2) . .
Al3 Al Uani 0.19790(4) 1.09664(4) 0.17402(2) 1.000 0.0258(2) . .
Al4 Al Uani 0.16283(4) 0.89936(4) 0.33023(2) 1.000 0.0252(2) . .
O1 O Uani 0.44507(9) 0.93540(9) 0.26261(5) 1.000 0.0252(4) . .
O2 O Uani 0.30941(9) 1.07771(9) 0.22014(5) 1.000 0.0243(3) . .
O3 O Uani 0.09829(9) 1.15505(10) 0.22270(6) 1.000 0.0290(4) . .
O4 O Uani 0.17791(9) 1.02521(9) 0.30709(5) 1.000 0.0235(3) . .
O5 O Uani 0.30819(9) 0.84699(9) 0.32704(5) 1.000 0.0245(3) . .
O6 O Uani 0.48259(10) 0.78506(11) 0.36132(6) 1.000 0.0336(4) . .
O7 O Uani 0.23948(9) 0.95213(10) 0.20255(5) 1.000 0.0249(4) . .
O8 O Uani 0.13892(10) 0.87302(11) 0.26111(6) 1.000 0.0313(4) . .
C1 C Uani 0.48577(14) 1.08276(15) 0.18554(9) 1.000 0.0303(6) . .
```

C2 C Uani 0.47023(16) 1.18361(17) 0.19383(10) 1.000 0.0398(7) . .
C3 C Uani 0.5183(2) 1.2379(2) 0.15535(14) 1.000 0.0607(10) . .
C4 C Uani 0.5795(2) 1.1945(2) 0.10947(14) 1.000 0.0669(11) . .
C5 C Uani 0.59587(19) 1.0958(2) 0.10133(11) 1.000 0.0521(8) . .
C6 C Uani 0.55085(15) 1.03812(17) 0.13913(9) 1.000 0.0358(6) . .
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C8 C Uani 0.3016(2) 1.3279(2) 0.21931(15) 1.000 0.0698(10) . .
C9 C Uani 0.4648(2) 1.2701(2) 0.28337(14) 1.000 0.0668(11) . .
C10 C Uani 0.56817(17) 0.92966(18) 0.12882(10) 1.000 0.0423(7) . .
C11 C Uani 0.6681(2) 0.8744(2) 0.09519(12) 1.000 0.0625(10) . .
C12 C Uani 0.4751(2) 0.9308(3) 0.09704(14) 1.000 0.0698(11) . .
C13 C Uani 0.03014(14) 1.20200(14) 0.32595(8) 1.000 0.0273(5) . .
C14 C Uani 0.07598(15) 1.22442(15) 0.37267(9) 1.000 0.0314(6) . .
C15 C Uani 0.01137(17) 1.28907(18) 0.41153(10) 1.000 0.0419(7) . .
C16 C Uani -0.09651(18) 1.33173(19) 0.40463(11) 1.000 0.0482(8) . .
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C18 C Uani -0.08081(14) 1.24817(15) 0.31888(9) 1.000 0.0313(6) . .
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C21 C Uani 0.2323(2) 1.0942(2) 0.43563(12) 1.000 0.0604(9) . .
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C24 C Uani -0.23701(17) 1.2197(2) 0.28540(12) 1.000 0.0520(8) . .
C25 C Uani 0.37221(14) 0.69640(14) 0.41888(8) 1.000 0.0263(5) . .
C26 C Uani 0.37156(14) 0.70859(15) 0.47945(8) 1.000 0.0299(5) . .
C27 C Uani 0.35922(16) 0.63380(17) 0.52382(9) 1.000 0.0377(6) . .
C28 C Uani 0.34938(17) 0.54807(18) 0.51028(10) 1.000 0.0430(7) . .
C29 C Uani 0.35138(17) 0.53463(16) 0.45128(10) 1.000 0.0395(7) . .
C30 C Uani 0.36248(15) 0.60811(15) 0.40532(9) 1.000 0.0310(6) . .
C31 C Uani 0.38857(16) 0.79946(16) 0.49653(9) 1.000 0.0356(6) . .
C32 C Uani 0.3209(2) 0.8454(2) 0.54845(11) 1.000 0.0531(8) . .
C33 C Uani 0.50451(18) 0.76472(19) 0.51184(11) 1.000 0.0460(8) . .
C34 C Uani 0.37219(17) 0.58576(16) 0.34175(10) 1.000 0.0374(7) . .
C35 C Uani 0.2855(2) 0.5561(2) 0.32480(13) 1.000 0.0593(10) . .
C36 C Uani 0.47974(18) 0.50019(19) 0.33275(11) 1.000 0.0470(8) . .
C37 C Uani 0.13271(16) 0.88098(16) 0.14711(9) 1.000 0.0334(6) . .
C38 C Uani 0.20473(18) 0.81243(19) 0.11154(10) 1.000 0.0436(7) . .
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C40 C Uani 0.0649(2) 0.8454(2) 0.04336(11) 1.000 0.0613(10) . .
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C44 C Uani -0.1314(2) 1.1060(2) 0.12759(13) 1.000 0.0655(10) . .
C45 C Uani -0.1152(2) 0.9520(3) 0.20419(14) 1.000 0.0696(11) . .
C46 C Uani 0.3201(2) 0.7518(2) 0.13029(12) 1.000 0.0581(9) . .
C47 C Uani 0.3936(3) 0.7254(3) 0.07745(17) 1.000 0.0896(16) . .
C48 C Uani 0.3344(3) 0.6545(3) 0.17237(18) 1.000 0.1098(17) . .
C49 C Uani 0.61611(16) 0.91290(18) 0.35492(9) 1.000 0.0381(7) . .
C50 C Uani 0.5252(2) 0.9900(2) 0.38619(12) 1.000 0.0553(9) . .
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C53 C Uani 0.65869(17) 0.71296(17) 0.27610(10) 1.000 0.0433(7) . .
C54 C Uani 0.7523(2) 0.7289(2) 0.24474(13) 1.000 0.0666(10) . .
C55 C Uani 0.7047(2) 0.6198(2) 0.32790(13) 1.000 0.0626(9) . .
C56 C Uani 0.6017(2) 0.6804(2) 0.23327(12) 1.000 0.0605(10) . .
C57 C Uani 0.17910(16) 1.16111(17) 0.08958(9) 1.000 0.0360(6) . .
C58 C Uani 0.2621(2) 1.2055(2) 0.07050(11) 1.000 0.0574(10) . .
C59 C Uani 0.18355(19) 1.0867(2) 0.04725(9) 1.000 0.0459(8) . .
C60 C Uani 0.0705(2) 1.2537(2) 0.08216(11) 1.000 0.0619(9) . .
C61 C Uani 0.06621(15) 0.88443(16) 0.39281(9) 1.000 0.0327(6) . .
C62 C Uani -0.04169(18) 0.9696(2) 0.37324(13) 1.000 0.0651(10) . .
C63 C Uani 0.0631(3) 0.7778(2) 0.39820(16) 1.000 0.0802(13) . .
C64 C Uani 0.0913(2) 0.8945(3) 0.45536(12) 1.000 0.0767(13) . .
B1 B Uani 0.41866(16) 1.03007(16) 0.22297(9) 1.000 0.0246(6) . .

B2 B Uani 0.10203(15) 1.12814(16) 0.28230(9) 1.000 0.0256(6) . .
 B3 B Uani 0.39259(16) 0.77740(16) 0.36801(9) 1.000 0.0252(6) . .
 B4 B Uani 0.17008(16) 0.89993(17) 0.20665(10) 1.000 0.0279(6) . .
 C65 C Uani 0.0148(3) 0.4803(4) 0.2448(4) 1.000 0.117(2) . .
 C66 C Uani 0.0358(3) 0.5502(6) 0.2728(2) 1.000 0.131(2) . .
 C67 C Uani 0.0471(3) 0.6336(4) 0.2359(4) 1.000 0.121(2) . .
 C68 C Uani 0.0380(4) 0.6437(5) 0.1806(3) 1.000 0.129(3) . .
 C69 C Uani 0.0169(5) 0.5804(6) 0.1549(3) 1.000 0.157(4) . .
 C70 C Uani 0.0070(4) 0.4982(4) 0.1872(4) 1.000 0.130(3) . .
 C71B C Uani 0.7243(5) 0.5128(6) -0.0434(2) 0.674(11) 0.218(9) . .
 C72B C Uani 0.8126(4) 0.4789(7) -0.0067(3) 0.674(11) 0.180(6) . .
 C73B C Uani 0.8022(4) 0.4707(10) 0.0549(3) 0.674(11) 0.355(12) . .
 C74B C Uani 0.7035(4) 0.4963(7) 0.0798(2) 0.674(11) 0.417(13) . .
 C75B C Uani 0.6151(4) 0.5302(5) 0.04306(19) 0.674(11) 0.64(3) . .
 C76B C Uani 0.6256(5) 0.5385(8) -0.01853(19) 0.674(11) 0.393(14) . .
 C77 C Uani 0.0692(2) 0.5229(2) 0.46222(13) 1.000 0.0606(10) . .
 C78 C Uani 0.1056(2) 0.4534(2) 0.51402(13) 1.000 0.0556(9) . .
 C79 C Uani -0.0361(2) 0.5695(2) 0.44813(13) 1.000 0.0616(10) . .
 C71A C Uani 0.7697(13) 0.4942(16) -0.0427(7) 0.326(11) 0.37(3) . .
 C72A C Uani 0.8439(12) 0.5146(15) -0.0155(7) 0.326(11) 0.72(10) . .
 C73A C Uani 0.8279(13) 0.5390(11) 0.0417(7) 0.326(11) 0.189(15) . .
 C74A C Uani 0.7376(15) 0.5430(11) 0.0719(7) 0.326(11) 0.226(17) . .
 C75A C Uani 0.6634(11) 0.5226(16) 0.0448(11) 0.326(11) 0.39(3) . .
 C76A C Uani 0.6794(10) 0.4982(17) -0.0125(11) 0.326(11) 0.51(5) . .
 H3 H Uiso 0.50867 1.30584 0.16093 1.000 0.0730 . .
 H4 H Uiso 0.61062 1.23305 0.08329 1.000 0.0802 . .
 H5 H Uiso 0.63836 1.06659 0.06956 1.000 0.0625 . .
 H7 H Uiso 0.38348 1.18258 0.27001 1.000 0.0543 . .
 H8 H Uiso 0.31849 1.37979 0.19187 1.000 0.1046 . .
 H8' H Uiso 0.26056 1.36016 0.25234 1.000 0.1046 . .
 H8" H Uiso 0.26049 1.30274 0.19788 1.000 0.1046 . .
 H9 H Uiso 0.52996 1.21002 0.29822 1.000 0.1000 . .
 H9' H Uiso 0.42190 1.29666 0.31723 1.000 0.1000 . .
 H9" H Uiso 0.48173 1.32542 0.25970 1.000 0.1000 . .
 H10 H Uiso 0.57501 0.88556 0.16908 1.000 0.0508 . .
 H11 H Uiso 0.66290 0.91340 0.05460 1.000 0.0938 . .
 H11' H Uiso 0.67644 0.80319 0.09328 1.000 0.0938 . .
 H11" H Uiso 0.72904 0.87110 0.11615 1.000 0.0938 . .
 H12 H Uiso 0.41191 0.95895 0.12063 1.000 0.1048 . .
 H12' H Uiso 0.48873 0.85929 0.09233 1.000 0.1048 . .
 H12" H Uiso 0.46458 0.97494 0.05761 1.000 0.1048 . .
 H15 H Uiso 0.04205 1.30379 0.44301 1.000 0.0503 . .
 H16 H Uiso -0.13962 1.37482 0.43165 1.000 0.0579 . .
 H17 H Uiso -0.21608 1.34279 0.35450 1.000 0.0517 . .
 H19 H Uiso 0.22847 1.15273 0.34588 1.000 0.0423 . .
 H20 H Uiso 0.20240 1.32553 0.35511 1.000 0.0891 . .
 H20' H Uiso 0.30694 1.23875 0.38952 1.000 0.0891 . .
 H20" H Uiso 0.20358 1.29388 0.42623 1.000 0.0891 . .
 H21 H Uiso 0.19693 1.12004 0.47160 1.000 0.0906 . .
 H21' H Uiso 0.30839 1.06910 0.44106 1.000 0.0906 . .
 H21" H Uiso 0.21589 1.03650 0.42861 1.000 0.0906 . .
 H22 H Uiso -0.08576 1.16721 0.25324 1.000 0.0431 . .
 H23 H Uiso -0.20345 1.38935 0.22920 1.000 0.0828 . .
 H23' H Uiso -0.19249 1.31300 0.18292 1.000 0.0828 . .
 H23" H Uiso -0.09140 1.32684 0.20203 1.000 0.0828 . .
 H24 H Uiso -0.22286 1.16390 0.32013 1.000 0.0780 . .
 H24' H Uiso -0.26316 1.20135 0.25196 1.000 0.0780 . .
 H24" H Uiso -0.28995 1.28555 0.29547 1.000 0.0780 . .
 H27 H Uiso 0.35757 0.64236 0.56440 1.000 0.0452 . .
 H28 H Uiso 0.34122 0.49800 0.54131 1.000 0.0516 . .
 H29 H Uiso 0.34513 0.47491 0.44206 1.000 0.0474 . .
 H31 H Uiso 0.36968 0.85644 0.46088 1.000 0.0428 . .
 H32 H Uiso 0.24795 0.85783 0.54118 1.000 0.0797 . .
 H32' H Uiso 0.32430 0.91164 0.55159 1.000 0.0797 . .

H32" H Uiso 0.34737 0.79591 0.58575 1.000 0.0797 . .
H33 H Uiso 0.52477 0.70974 0.54723 1.000 0.0690 . .
H33' H Uiso 0.51581 0.82465 0.52001 1.000 0.0690 . .
H33" H Uiso 0.54734 0.73747 0.47809 1.000 0.0690 . .
H34 H Uiso 0.36555 0.65117 0.31415 1.000 0.0448 . .
H35 H Uiso 0.28907 0.49304 0.35191 1.000 0.0889 . .
H35' H Uiso 0.29498 0.54231 0.28367 1.000 0.0889 . .
H35" H Uiso 0.21683 0.61377 0.32795 1.000 0.0889 . .
H36 H Uiso 0.53467 0.52050 0.34315 1.000 0.0705 . .
H36' H Uiso 0.48629 0.49056 0.29088 1.000 0.0705 . .
H36" H Uiso 0.48745 0.43447 0.35843 1.000 0.0705 . .
H39 H Uiso 0.21669 0.74958 0.03624 1.000 0.0688 . .
H40 H Uiso 0.04160 0.83269 0.00833 1.000 0.0734 . .
H41 H Uiso -0.07778 0.94869 0.06458 1.000 0.0637 . .
H43 H Uiso -0.01701 1.02710 0.19325 1.000 0.0499 . .
H44 H Uiso -0.17226 1.08836 0.10120 1.000 0.0983 . .
H44' H Uiso -0.09190 1.14119 0.10348 1.000 0.0983 . .
H44" H Uiso -0.17916 1.15272 0.15347 1.000 0.0983 . .
H45 H Uiso -0.15279 0.92944 0.17855 1.000 0.1043 . .
H45' H Uiso -0.16576 1.00059 0.22817 1.000 0.1043 . .
H45" H Uiso -0.06589 0.89080 0.23071 1.000 0.1043 . .
H46 H Uiso 0.34035 0.79635 0.15196 1.000 0.0696 . .
H47 H Uiso 0.46656 0.69991 0.09128 1.000 0.1344 . .
H47' H Uiso 0.37640 0.78840 0.04709 1.000 0.1344 . .
H47" H Uiso 0.38482 0.67110 0.06016 1.000 0.1344 . .
H48 H Uiso 0.28856 0.67225 0.20656 1.000 0.1643 . .
H48' H Uiso 0.40778 0.61806 0.18640 1.000 0.1643 . .
H48" H Uiso 0.31623 0.60882 0.15194 1.000 0.1643 . .
H50 H Uiso 0.55237 1.02545 0.40963 1.000 0.0829 . .
H50' H Uiso 0.49096 0.95188 0.41275 1.000 0.0829 . .
H50" H Uiso 0.47413 1.04206 0.35621 1.000 0.0829 . .
H51 H Uiso 0.75735 0.78682 0.38420 1.000 0.0838 . .
H51' H Uiso 0.66657 0.80090 0.43219 1.000 0.0838 . .
H51" H Uiso 0.72477 0.87799 0.42343 1.000 0.0838 . .
H52 H Uiso 0.61849 1.02268 0.28229 1.000 0.0798 . .
H52' H Uiso 0.72910 0.92338 0.29443 1.000 0.0798 . .
H52" H Uiso 0.69343 1.01098 0.33630 1.000 0.0798 . .
H54 H Uiso 0.79526 0.66735 0.22664 1.000 0.0998 . .
H54' H Uiso 0.79503 0.73823 0.27402 1.000 0.0998 . .
H54" H Uiso 0.72625 0.79115 0.21359 1.000 0.0998 . .
H55 H Uiso 0.64734 0.60647 0.34887 1.000 0.0939 . .
H55' H Uiso 0.74388 0.63640 0.35582 1.000 0.0939 . .
H55" H Uiso 0.75190 0.55725 0.31189 1.000 0.0939 . .
H56 H Uiso 0.65131 0.61659 0.21936 1.000 0.0908 . .
H56' H Uiso 0.57296 0.73672 0.19895 1.000 0.0908 . .
H56" H Uiso 0.54431 0.66706 0.25413 1.000 0.0908 . .
H58 H Uiso 0.33223 1.14778 0.07335 1.000 0.0861 . .
H58' H Uiso 0.25910 1.25406 0.09686 1.000 0.0861 . .
H58" H Uiso 0.24738 1.24256 0.02920 1.000 0.0861 . .
H59 H Uiso 0.13148 1.05795 0.05902 1.000 0.0689 . .
H59' H Uiso 0.25389 1.02942 0.04941 1.000 0.0689 . .
H59" H Uiso 0.16813 1.12524 0.00627 1.000 0.0689 . .
H60 H Uiso 0.05881 1.28820 0.04032 1.000 0.0929 . .
H60' H Uiso 0.06723 1.30384 0.10751 1.000 0.0929 . .
H60" H Uiso 0.01610 1.22801 0.09392 1.000 0.0929 . .
H62 H Uiso -0.09385 0.96290 0.40219 1.000 0.0976 . .
H62' H Uiso -0.06020 0.96242 0.33384 1.000 0.0976 . .
H62" H Uiso -0.04058 1.03847 0.37105 1.000 0.0976 . .
H63 H Uiso 0.00448 0.77641 0.42334 1.000 0.1204 . .
H63' H Uiso 0.12924 0.72334 0.41632 1.000 0.1204 . .
H63" H Uiso 0.05364 0.76507 0.35842 1.000 0.1204 . .
H64 H Uiso 0.08742 0.96492 0.45490 1.000 0.1151 . .
H64' H Uiso 0.16229 0.84243 0.46777 1.000 0.1151 . .
H64" H Uiso 0.04039 0.88262 0.48351 1.000 0.1151 . .

H65 H Uiso 0.00665 0.42157 0.26750 1.000 0.1399 . .
 H66 H Uiso 0.04203 0.54089 0.31504 1.000 0.1577 . .
 H67 H Uiso 0.06169 0.68283 0.25274 1.000 0.1459 . .
 H68 H Uiso 0.04703 0.70071 0.15622 1.000 0.1558 . .
 H69 H Uiso 0.00852 0.59288 0.11271 1.000 0.1886 . .
 H70 H Uiso -0.00625 0.45115 0.16743 1.000 0.1553 . .
 H71B H Uiso 0.73141 0.51845 -0.08552 0.674(11) 0.2608 . .
 H72B H Uiso 0.88007 0.46138 -0.02375 0.674(11) 0.2165 . .
 H73B H Uiso 0.86253 0.44750 0.07993 0.674(11) 0.4273 . .
 H74B H Uiso 0.69634 0.49070 0.12184 0.674(11) 0.4959 . .
 H75B H Uiso 0.54767 0.54777 0.06007 0.674(11) 0.7701 . .
 H76B H Uiso 0.56521 0.56165 -0.04361 0.674(11) 0.4698 . .
 H77 H Uiso 0.11716 0.53896 0.43574 1.000 0.0727 . .
 H78 H Uiso 0.17864 0.42127 0.52370 1.000 0.0668 . .
 H79 H Uiso -0.06083 0.61790 0.41204 1.000 0.0738 . .
 H71 H Uiso 0.78061 0.47756 -0.08184 0.326(11) 0.4462 . .
 H72 H Uiso 0.90565 0.51191 -0.03616 0.326(11) 0.8638 . .
 H73 H Uiso 0.87870 0.55295 0.06030 0.326(11) 0.2279 . .
 H74 H Uiso 0.72670 0.55965 0.11107 0.326(11) 0.2705 . .
 H75 H Uiso 0.60165 0.52530 0.06538 0.326(11) 0.4744 . .
 H76 H Uiso 0.62861 0.48425 -0.03107 0.326(11) 0.6195 . .

loop_

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Al1 0.0199(2) 0.0230(3) 0.0209(3) -0.0037(2) 0.0007(2) -0.0092(2)
 Al2 0.0206(3) 0.0309(3) 0.0309(3) -0.0018(2) -0.0011(2) -0.0095(2)
 Al3 0.0231(3) 0.0313(3) 0.0214(3) -0.0020(2) -0.0005(2) -0.0105(2)
 Al4 0.0235(3) 0.0277(3) 0.0249(3) -0.0028(2) 0.0022(2) -0.0119(2)
 O1 0.0209(6) 0.0264(7) 0.0277(7) -0.0027(5) 0.0003(5) -0.0099(5)
 O2 0.0222(6) 0.0255(6) 0.0264(6) -0.0021(5) -0.0002(5) -0.0118(5)
 O3 0.0227(6) 0.0312(7) 0.0266(7) -0.0019(5) 0.0000(5) -0.0060(5)
 O4 0.0225(6) 0.0237(6) 0.0234(6) -0.0047(5) 0.0030(5) -0.0087(5)
 O5 0.0224(6) 0.0234(6) 0.0256(6) -0.0013(5) -0.0001(5) -0.0085(5)
 O6 0.0273(7) 0.0400(8) 0.0311(7) 0.0037(6) -0.0030(5) -0.0150(6)
 O7 0.0246(6) 0.0303(7) 0.0226(6) -0.0062(5) 0.0007(5) -0.0134(5)
 O8 0.0324(7) 0.0391(8) 0.0290(7) -0.0061(6) 0.0006(5) -0.0210(6)
 C1 0.0234(9) 0.0340(10) 0.0323(10) 0.0010(8) -0.0014(7) -0.0130(8)
 C2 0.0337(10) 0.0360(11) 0.0518(13) -0.0016(10) 0.0039(9) -0.0190(9)
 C3 0.0559(15) 0.0443(14) 0.086(2) -0.0004(14) 0.0167(14) -0.0306(13)
 C4 0.0599(17) 0.0633(18) 0.077(2) 0.0080(15) 0.0223(15) -0.0351(15)
 C5 0.0429(13) 0.0605(16) 0.0480(14) 0.0023(12) 0.0155(11) -0.0228(12)
 C6 0.0277(10) 0.0435(12) 0.0326(11) 0.0015(9) 0.0019(8) -0.0145(9)
 C7 0.0425(12) 0.0371(12) 0.0646(16) -0.0158(11) 0.0083(11) -0.0228(10)
 C8 0.0512(16) 0.0548(17) 0.093(2) -0.0205(16) 0.0090(15) -0.0096(13)
 C9 0.0671(18) 0.0617(18) 0.094(2) -0.0335(16) 0.0058(16) -0.0410(15)
 C10 0.0404(12) 0.0493(13) 0.0358(12) -0.0103(10) 0.0122(9) -0.0172(10)
 C11 0.0575(16) 0.0728(19) 0.0512(16) -0.0191(14) 0.0254(13) -0.0206(14)
 C12 0.0639(18) 0.084(2) 0.074(2) -0.0338(17) 0.0078(15) -0.0357(17)
 C13 0.0272(9) 0.0239(9) 0.0287(10) -0.0043(7) 0.0035(7) -0.0089(7)
 C14 0.0320(10) 0.0287(10) 0.0325(10) -0.0073(8) 0.0029(8) -0.0110(8)
 C15 0.0419(12) 0.0428(12) 0.0411(12) -0.0189(10) 0.0065(9) -0.0137(10)
 C16 0.0398(12) 0.0518(14) 0.0532(14) -0.0287(12) 0.0152(10) -0.0130(11)
 C17 0.0293(10) 0.0386(12) 0.0556(14) -0.0163(10) 0.0089(10) -0.0059(9)
 C18 0.0264(9) 0.0279(10) 0.0357(11) -0.0056(8) 0.0033(8) -0.0077(8)
 C19 0.0318(10) 0.0367(11) 0.0375(11) -0.0151(9) 0.0013(8) -0.0111(9)
 C20 0.0470(14) 0.0596(16) 0.083(2) -0.0276(15) 0.0044(13) -0.0277(13)
 C21 0.0498(15) 0.0617(17) 0.0546(16) 0.0024(13) -0.0122(12) -0.0115(13)
 C22 0.0248(9) 0.0395(11) 0.0405(12) -0.0079(9) 0.0028(8) -0.0102(8)

C23 0.0556(15) 0.0572(16) 0.0476(14) 0.0022(12) -0.0096(12) -0.0212(13)
 C24 0.0305(11) 0.0653(16) 0.0633(16) -0.0183(13) 0.0051(10) -0.0203(11)
 C25 0.0233(8) 0.0250(9) 0.0273(9) -0.0013(7) -0.0014(7) -0.0078(7)
 C26 0.0268(9) 0.0317(10) 0.0261(9) -0.0028(8) 0.0012(7) -0.0081(8)
 C27 0.0367(11) 0.0430(12) 0.0274(10) 0.0012(9) 0.0024(8) -0.0137(9)
 C28 0.0399(12) 0.0399(12) 0.0425(13) 0.0109(10) 0.0016(9) -0.0171(10)
 C29 0.0397(11) 0.0286(10) 0.0487(13) 0.0025(9) -0.0042(10) -0.0156(9)
 C30 0.0312(10) 0.0258(10) 0.0338(10) -0.0022(8) -0.0036(8) -0.0102(8)
 C31 0.0430(11) 0.0347(11) 0.0264(10) -0.0064(8) -0.0004(8) -0.0128(9)
 C32 0.0551(15) 0.0637(16) 0.0412(13) -0.0266(12) 0.0050(11) -0.0187(13)
 C33 0.0472(13) 0.0504(14) 0.0463(13) -0.0096(11) -0.0020(10) -0.0250(11)
 C34 0.0473(12) 0.0262(10) 0.0389(12) -0.0059(9) -0.0062(9) -0.0145(9)
 C35 0.0506(14) 0.0673(18) 0.0668(18) -0.0299(14) -0.0075(13) -0.0229(13)
 C36 0.0480(13) 0.0437(13) 0.0496(14) -0.0142(11) 0.0039(11) -0.0171(11)
 C37 0.0364(10) 0.0407(11) 0.0310(10) -0.0082(9) -0.0005(8) -0.0227(9)
 C38 0.0448(12) 0.0529(14) 0.0416(12) -0.0194(11) 0.0007(10) -0.0241(11)
 C39 0.0625(16) 0.0756(19) 0.0446(14) -0.0337(13) 0.0054(12) -0.0304(14)
 C40 0.0689(17) 0.084(2) 0.0410(14) -0.0239(14) -0.0130(12) -0.0344(16)
 C41 0.0520(14) 0.0688(17) 0.0448(14) -0.0133(12) -0.0133(11) -0.0279(13)
 C42 0.0394(11) 0.0482(13) 0.0337(11) -0.0070(9) -0.0041(9) -0.0258(10)
 C43 0.0314(10) 0.0563(14) 0.0416(12) -0.0135(10) -0.0037(9) -0.0200(10)
 C44 0.0511(15) 0.0677(19) 0.0648(18) -0.0119(15) -0.0073(13) -0.0106(14)
 C45 0.0596(17) 0.086(2) 0.0709(19) -0.0138(16) 0.0194(14) -0.0396(17)
 C46 0.0452(14) 0.0665(18) 0.0641(17) -0.0403(15) -0.0006(12) -0.0131(12)
 C47 0.063(2) 0.116(3) 0.103(3) -0.061(2) 0.0243(18) -0.036(2)
 C48 0.080(3) 0.117(3) 0.094(3) 0.026(2) -0.025(2) -0.017(2)
 C49 0.0332(10) 0.0474(13) 0.0385(12) -0.0052(10) -0.0039(9) -0.0216(10)
 C50 0.0573(15) 0.0591(16) 0.0580(16) -0.0233(13) 0.0019(12) -0.0273(13)
 C51 0.0486(14) 0.0717(18) 0.0498(15) 0.0011(13) -0.0163(11) -0.0297(13)
 C52 0.0517(14) 0.0640(16) 0.0572(15) -0.0005(12) -0.0067(12) -0.0397(13)
 C53 0.0345(11) 0.0365(12) 0.0469(13) -0.0041(10) 0.0018(9) -0.0043(9)
 C54 0.0375(13) 0.0713(19) 0.0700(19) -0.0137(15) 0.0156(12) -0.0031(13)
 C55 0.0590(16) 0.0378(14) 0.0679(18) -0.0008(12) -0.0062(14) 0.0002(12)
 C56 0.0790(19) 0.0432(14) 0.0563(16) -0.0140(12) -0.0012(14) -0.0199(14)
 C57 0.0369(11) 0.0443(12) 0.0251(10) 0.0002(9) -0.0015(8) -0.0171(9)
 C58 0.0739(18) 0.0726(18) 0.0371(13) 0.0078(12) -0.0038(12) -0.0476(15)
 C59 0.0513(13) 0.0656(16) 0.0258(11) -0.0036(10) -0.0022(9) -0.0303(12)
 C60 0.0583(16) 0.0605(17) 0.0403(14) 0.0076(12) -0.0094(12) -0.0036(13)
 C61 0.0280(9) 0.0344(11) 0.0334(10) -0.0035(8) 0.0088(8) -0.0126(8)
 C62 0.0316(12) 0.0684(18) 0.0742(19) 0.0133(15) 0.0105(12) -0.0111(12)
 C63 0.089(2) 0.0555(18) 0.106(3) -0.0209(17) 0.061(2) -0.0437(17)
 C64 0.0591(18) 0.129(3) 0.0474(16) -0.0306(18) 0.0192(13) -0.0401(19)
 B1 0.0254(10) 0.0292(11) 0.0216(10) -0.0064(8) 0.0008(7) -0.0130(8)
 B2 0.0215(9) 0.0267(10) 0.0282(10) -0.0051(8) 0.0017(8) -0.0094(8)
 B3 0.0274(10) 0.0228(10) 0.0232(10) -0.0060(8) 0.0003(8) -0.0075(8)
 B4 0.0255(10) 0.0300(11) 0.0299(11) -0.0089(9) 0.0001(8) -0.0117(8)
 C65 0.054(2) 0.078(3) 0.188(6) 0.038(4) 0.000(3) -0.021(2)
 C66 0.053(2) 0.178(6) 0.093(3) 0.000(4) -0.022(2) 0.014(3)
 C67 0.067(2) 0.082(3) 0.211(6) -0.054(4) -0.049(3) -0.009(2)
 C68 0.104(4) 0.130(5) 0.175(6) 0.016(4) -0.004(4) -0.084(3)
 C69 0.173(6) 0.220(8) 0.121(5) -0.059(5) 0.065(4) -0.119(6)
 C70 0.138(4) 0.089(3) 0.188(6) -0.072(4) 0.050(4) -0.059(3)
 C71B 0.37(2) 0.225(17) 0.115(8) 0.029(9) -0.026(12) -0.198(17)
 C72B 0.167(10) 0.213(13) 0.094(7) -0.020(7) 0.018(7) -0.017(9)
 C73B 0.144(11) 0.42(3) 0.212(15) 0.156(18) -0.011(10) 0.085(14)
 C74B 0.25(2) 0.49(3) 0.188(15) 0.152(18) -0.076(15) 0.09(2)
 C75B 0.25(3) 0.86(6) 0.38(4) -0.19(4) 0.11(3) 0.22(3)
 C76B 0.28(2) 0.32(2) 0.36(3) -0.21(2) -0.14(2) 0.166(19)
 C77 0.0588(16) 0.0511(16) 0.0720(19) -0.0072(14) 0.0143(14) -0.0256(13)
 C78 0.0482(14) 0.0464(14) 0.0704(18) -0.0100(13) -0.0087(13) -0.0165(12)
 C79 0.0676(18) 0.0512(16) 0.0572(17) 0.0026(13) -0.0025(14) -0.0202(14)
 C71A 0.157(19) 0.13(2) 0.78(8) -0.23(3) -0.26(4) 0.079(15)
 C72A 1.4(3) 0.080(18) 0.51(9) -0.06(3) -0.44(13) -0.09(6)
 C73A 0.24(3) 0.117(16) 0.19(3) 0.107(17) -0.11(2) -0.091(18)

C74A 0.21(3) 0.107(13) 0.36(4) -0.104(19) 0.21(3) -0.064(16)
 C75A 0.088(14) 0.60(9) 0.35(5) -0.24(5) 0.15(2) 0.04(3)
 C76A 0.124(19) 0.55(7) 1.06(13) -0.73(9) 0.21(4) -0.12(3)

#=====

10. MOLECULAR GEOMETRY

_geom_special_details

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

;

loop_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_1

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Al1	Al4	2.6650(8)	.	.	yes
Al1	O1	1.8688(15)	.	.	yes
Al1	O2	1.9244(13)	.	.	yes
Al1	O4	1.8671(14)	.	.	yes
Al1	O5	1.8233(13)	.	.	yes
Al1	O7	1.8511(13)	.	.	yes
Al1	B1	2.376(2)	.	.	yes
Al2	O1	1.9400(14)	.	.	yes
Al2	O6	1.7612(16)	.	.	yes
Al2	C49	1.990(2)	.	.	yes
Al2	C53	1.984(2)	.	.	yes
Al3	O2	1.8274(14)	.	.	yes
Al3	O3	1.7474(15)	.	.	yes
Al3	O7	1.8903(14)	.	.	yes
Al3	C57	1.959(2)	.	.	yes
Al4	O4	1.8732(13)	.	.	yes
Al4	O5	1.8555(15)	.	.	yes
Al4	O8	1.7590(15)	.	.	yes
Al4	C61	1.956(2)	.	.	yes
O1	B1	1.401(2)	.	.	yes
O2	B1	1.391(3)	.	.	yes
O3	B2	1.340(2)	.	.	yes
O4	B2	1.440(2)	.	.	yes
O5	B3	1.438(3)	.	.	yes
O6	B3	1.308(3)	.	.	yes
O7	B4	1.440(3)	.	.	yes
O8	B4	1.336(3)	.	.	yes
C1	C2	1.406(3)	.	.	no
C1	C6	1.414(3)	.	.	no
C1	B1	1.565(3)	.	.	yes
C2	C3	1.396(4)	.	.	no
C2	C7	1.529(3)	.	.	no
C3	C4	1.376(4)	.	.	no
C4	C5	1.372(4)	.	.	no
C5	C6	1.392(3)	.	.	no
C6	C10	1.520(3)	.	.	no
C7	C8	1.529(4)	.	.	no
C7	C9	1.540(4)	.	.	no
C10	C11	1.530(4)	.	.	no
C10	C12	1.517(4)	.	.	no

C13	C14	1.417(3)	.	.	no
C13	C18	1.418(3)	.	.	no
C13	B2	1.576(3)	.	.	yes
C14	C15	1.398(3)	.	.	no
C14	C19	1.523(3)	.	.	no
C15	C16	1.380(4)	.	.	no
C16	C17	1.370(4)	.	.	no
C17	C18	1.397(3)	.	.	no
C18	C22	1.524(3)	.	.	no
C19	C20	1.524(4)	.	.	no
C19	C21	1.525(3)	.	.	no
C22	C23	1.528(3)	.	.	no
C22	C24	1.534(4)	.	.	no
C25	C26	1.418(3)	.	.	no
C25	C30	1.407(3)	.	.	no
C25	B3	1.588(3)	.	.	yes
C26	C27	1.393(3)	.	.	no
C26	C31	1.526(3)	.	.	no
C27	C28	1.372(3)	.	.	no
C28	C29	1.386(3)	.	.	no
C29	C30	1.395(3)	.	.	no
C30	C34	1.522(3)	.	.	no
C31	C32	1.534(3)	.	.	no
C31	C33	1.528(4)	.	.	no
C34	C35	1.528(4)	.	.	no
C34	C36	1.524(3)	.	.	no
C37	C38	1.412(3)	.	.	no
C37	C42	1.407(3)	.	.	no
C37	B4	1.582(3)	.	.	yes
C38	C39	1.394(4)	.	.	no
C38	C46	1.524(4)	.	.	no
C39	C40	1.363(4)	.	.	no
C40	C41	1.376(4)	.	.	no
C41	C42	1.398(3)	.	.	no
C42	C43	1.518(3)	.	.	no
C43	C44	1.522(4)	.	.	no
C43	C45	1.511(4)	.	.	no
C46	C47	1.532(5)	.	.	no
C46	C48	1.484(5)	.	.	no
C49	C50	1.531(4)	.	.	no
C49	C51	1.542(3)	.	.	no
C49	C52	1.531(4)	.	.	no
C53	C54	1.539(4)	.	.	no
C53	C55	1.545(4)	.	.	no
C53	C56	1.534(4)	.	.	no
C57	C58	1.549(4)	.	.	no
C57	C59	1.534(3)	.	.	no
C57	C60	1.536(4)	.	.	no
C61	C62	1.520(4)	.	.	no
C61	C63	1.521(4)	.	.	no
C61	C64	1.529(4)	.	.	no
C3	H3	0.9508	.	.	no
C4	H4	0.9500	.	.	no
C5	H5	0.9498	.	.	no
C7	H7	1.0000	.	.	no
C8	H8	0.9797	.	.	no
C8	H8'	0.9800	.	.	no
C8	H8''	0.9804	.	.	no
C9	H9	0.9802	.	.	no
C9	H9'	0.9798	.	.	no
C9	H9''	0.9799	.	.	no
C10	H10	1.0000	.	.	no
C11	H11	0.9798	.	.	no
C11	H11'	0.9804	.	.	no

C11	H11"	0.9801	.	.	no
C12	H12	0.9799	.	.	no
C12	H12'	0.9799	.	.	no
C12	H12"	0.9802	.	.	no
C15	H15	0.9500	.	.	no
C16	H16	0.9501	.	.	no
C17	H17	0.9501	.	.	no
C19	H19	1.0001	.	.	no
C20	H20	0.9801	.	.	no
C20	H20'	0.9800	.	.	no
C20	H20"	0.9801	.	.	no
C21	H21	0.9799	.	.	no
C21	H21'	0.9797	.	.	no
C21	H21"	0.9806	.	.	no
C22	H22	1.0001	.	.	no
C23	H23	0.9799	.	.	no
C23	H23'	0.9798	.	.	no
C23	H23"	0.9804	.	.	no
C24	H24	0.9802	.	.	no
C24	H24'	0.9803	.	.	no
C24	H24"	0.9798	.	.	no
C27	H27	0.9500	.	.	no
C28	H28	0.9500	.	.	no
C29	H29	0.9499	.	.	no
C31	H31	1.0000	.	.	no
C32	H32	0.9796	.	.	no
C32	H32'	0.9796	.	.	no
C32	H32"	0.9803	.	.	no
C33	H33	0.9801	.	.	no
C33	H33'	0.9799	.	.	no
C33	H33"	0.9801	.	.	no
C34	H34	1.0001	.	.	no
C35	H35	0.9805	.	.	no
C35	H35'	0.9803	.	.	no
C35	H35"	0.9798	.	.	no
C36	H36	0.9801	.	.	no
C36	H36'	0.9800	.	.	no
C36	H36"	0.9800	.	.	no
C39	H39	0.9499	.	.	no
C40	H40	0.9499	.	.	no
C41	H41	0.9504	.	.	no
C43	H43	1.0000	.	.	no
C44	H44	0.9803	.	.	no
C44	H44'	0.9796	.	.	no
C44	H44"	0.9803	.	.	no
C45	H45	0.9801	.	.	no
C45	H45'	0.9801	.	.	no
C45	H45"	0.9799	.	.	no
C46	H46	1.0006	.	.	no
C47	H47	0.9800	.	.	no
C47	H47'	0.9803	.	.	no
C47	H47"	0.9797	.	.	no
C48	H48	0.9800	.	.	no
C48	H48'	0.9800	.	.	no
C48	H48"	0.9805	.	.	no
C50	H50	0.9802	.	.	no
C50	H50'	0.9799	.	.	no
C50	H50"	0.9799	.	.	no
C51	H51	0.9801	.	.	no
C51	H51'	0.9798	.	.	no
C51	H51"	0.9805	.	.	no
C52	H52	0.9796	.	.	no
C52	H52'	0.9804	.	.	no
C52	H52"	0.9803	.	.	no

C54	H54	0.9803	.	.	no
C54	H54'	0.9798	.	.	no
C54	H54"	0.9797	.	.	no
C55	H55	0.9810	.	.	no
C55	H55'	0.9793	.	.	no
C55	H55"	0.9803	.	.	no
C56	H56	0.9800	.	.	no
C56	H56'	0.9801	.	.	no
C56	H56"	0.9804	.	.	no
C58	H58	0.9800	.	.	no
C58	H58'	0.9792	.	.	no
C58	H58"	0.9799	.	.	no
C59	H59	0.9799	.	.	no
C59	H59'	0.9799	.	.	no
C59	H59"	0.9801	.	.	no
C60	H60	0.9798	.	.	no
C60	H60'	0.9796	.	.	no
C60	H60"	0.9806	.	.	no
C62	H62	0.9798	.	.	no
C62	H62'	0.9800	.	.	no
C62	H62"	0.9804	.	.	no
C63	H63	0.9797	.	.	no
C63	H63'	0.9800	.	.	no
C63	H63"	0.9798	.	.	no
C64	H64	0.9802	.	.	no
C64	H64'	0.9803	.	.	no
C64	H64"	0.9797	.	.	no
C65	C66	1.404(9)	.	.	no
C65	C70	1.292(13)	.	.	no
C66	C67	1.391(9)	.	.	no
C67	C68	1.248(11)	.	.	no
C68	C69	1.292(10)	.	.	no
C69	C70	1.324(10)	.	.	no
C65	H65	0.9494	.	.	no
C66	H66	0.9504	.	.	no
C67	H67	0.9501	.	.	no
C68	H68	0.9503	.	.	no
C69	H69	0.9494	.	.	no
C70	H70	0.9511	.	.	no
C71B	C72B	1.390(10)	.	.	no
C71B	C76B	1.389(11)	.	.	no
C72B	C73B	1.390(10)	.	.	no
C73B	C74B	1.390(11)	.	.	no
C74B	C75B	1.392(9)	.	.	no
C75B	C76B	1.390(6)	.	.	no
C71B	H71B	0.9506	.	.	no
C72B	H72B	0.9503	.	.	no
C73B	H73B	0.9490	.	.	no
C74B	H74B	0.9489	.	.	no
C75B	H75B	0.9494	.	.	no
C76B	H76B	0.9505	.	.	no
C77	C78	1.365(4)	.	.	no
C77	C79	1.371(4)	.	.	no
C78	C79	1.367(4)	.	2_566	no
C77	H77	0.9497	.	.	no
C78	H78	0.9504	.	.	no
C79	H79	0.9501	.	.	no
C71A	C72A	1.39(3)	.	.	no
C71A	C76A	1.39(3)	.	.	no
C72A	C73A	1.39(2)	.	.	no
C73A	C74A	1.39(3)	.	.	no
C74A	C75A	1.39(3)	.	.	no
C75A	C76A	1.39(3)	.	.	no
C71A	H71	0.9494	.	.	no

C72A	H72	0.9511	.	.	no
C73A	H73	0.9511	.	.	no
C74A	H74	0.9502	.	.	no
C75A	H75	0.9502	.	.	no
C76A	H76	0.9506	.	.	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					
Al4	Al1	O1	147.57(4)	.	yes
Al4	Al1	O2	138.55(5)	.	yes
Al4	Al1	O4	44.65(4)	.	yes
Al4	Al1	O5	44.06(5)	.	yes
Al4	Al1	O7	85.30(5)	.	yes
Al4	Al1	B1	171.42(6)	.	yes
O1	Al1	O2	71.86(6)	.	yes
O1	Al1	O4	145.24(6)	.	yes
O1	Al1	O5	104.00(6)	.	yes
O1	Al1	O7	116.00(6)	.	yes
O1	Al1	B1	36.11(6)	.	yes
O2	Al1	O4	97.24(6)	.	yes
O2	Al1	O5	170.85(6)	.	yes
O2	Al1	O7	81.48(6)	.	yes
O2	Al1	B1	35.85(7)	.	yes
O4	Al1	O5	81.54(6)	.	yes
O4	Al1	O7	93.89(6)	.	yes
O4	Al1	B1	127.08(7)	.	yes
O5	Al1	O7	107.63(6)	.	yes
O5	Al1	B1	139.92(7)	.	yes
O7	Al1	B1	98.52(7)	.	yes
O1	Al2	O6	94.56(7)	.	yes
O1	Al2	C49	106.53(8)	.	yes
O1	Al2	C53	114.94(8)	.	yes
O6	Al2	C49	110.79(8)	.	yes
O6	Al2	C53	105.98(9)	.	yes
C49	Al2	C53	120.87(11)	.	yes
O2	Al3	O3	97.69(6)	.	yes
O2	Al3	O7	83.03(6)	.	yes
O2	Al3	C57	123.29(9)	.	yes
O3	Al3	O7	102.75(6)	.	yes
O3	Al3	C57	117.73(9)	.	yes
O7	Al3	C57	124.81(8)	.	yes
Al1	Al4	O4	44.47(4)	.	yes
Al1	Al4	O5	43.10(4)	.	yes
Al1	Al4	O8	84.15(5)	.	yes
Al1	Al4	C61	160.77(7)	.	yes
O4	Al4	O5	80.54(6)	.	yes
O4	Al4	O8	101.69(6)	.	yes
O4	Al4	C61	121.65(8)	.	yes
O5	Al4	O8	98.16(7)	.	yes
O5	Al4	C61	133.09(8)	.	yes
O8	Al4	C61	114.19(9)	.	yes
Al1	O1	Al2	126.10(7)	.	yes
Al1	O1	B1	92.06(12)	.	yes
Al2	O1	B1	139.80(14)	.	yes
Al1	O2	Al3	92.52(6)	.	yes
Al1	O2	B1	90.05(11)	.	yes
Al3	O2	B1	141.53(12)	.	yes

A13	O3	B2	125.92(13)	.	.	.	yes
A11	O4	A14	90.88(6)	.	.	.	yes
A11	O4	B2	122.87(11)	.	.	.	yes
A14	O4	B2	130.40(13)	.	.	.	yes
A11	O5	A14	92.84(6)	.	.	.	yes
A11	O5	B3	128.38(13)	.	.	.	yes
A14	O5	B3	134.17(12)	.	.	.	yes
A12	O6	B3	146.31(14)	.	.	.	yes
A11	O7	A13	92.88(6)	.	.	.	yes
A11	O7	B4	120.77(12)	.	.	.	yes
A13	O7	B4	124.18(12)	.	.	.	yes
A14	O8	B4	129.56(15)	.	.	.	yes
C2	C1	C6	119.3(2)	.	.	.	no
C2	C1	B1	118.14(18)	.	.	.	yes
C6	C1	B1	122.05(18)	.	.	.	yes
C1	C2	C3	119.1(2)	.	.	.	no
C1	C2	C7	122.3(2)	.	.	.	no
C3	C2	C7	118.6(2)	.	.	.	no
C2	C3	C4	121.0(2)	.	.	.	no
C3	C4	C5	120.4(3)	.	.	.	no
C4	C5	C6	120.7(2)	.	.	.	no
C1	C6	C5	119.5(2)	.	.	.	no
C1	C6	C10	120.42(19)	.	.	.	no
C5	C6	C10	120.0(2)	.	.	.	no
C2	C7	C8	111.2(2)	.	.	.	no
C2	C7	C9	111.9(2)	.	.	.	no
C8	C7	C9	111.0(2)	.	.	.	no
C6	C10	C11	114.6(2)	.	.	.	no
C6	C10	C12	112.2(2)	.	.	.	no
C11	C10	C12	108.8(2)	.	.	.	no
C14	C13	C18	118.88(18)	.	.	.	no
C14	C13	B2	120.15(18)	.	.	.	yes
C18	C13	B2	120.97(17)	.	.	.	yes
C13	C14	C15	119.6(2)	.	.	.	no
C13	C14	C19	122.75(18)	.	.	.	no
C15	C14	C19	117.61(19)	.	.	.	no
C14	C15	C16	120.7(2)	.	.	.	no
C15	C16	C17	120.3(2)	.	.	.	no
C16	C17	C18	121.4(2)	.	.	.	no
C13	C18	C17	119.14(19)	.	.	.	no
C13	C18	C22	121.81(18)	.	.	.	no
C17	C18	C22	119.0(2)	.	.	.	no
C14	C19	C20	112.85(19)	.	.	.	no
C14	C19	C21	110.98(19)	.	.	.	no
C20	C19	C21	110.3(2)	.	.	.	no
C18	C22	C23	109.87(19)	.	.	.	no
C18	C22	C24	113.75(18)	.	.	.	no
C23	C22	C24	110.0(2)	.	.	.	no
C26	C25	C30	119.13(17)	.	.	.	no
C26	C25	B3	119.67(17)	.	.	.	yes
C30	C25	B3	121.03(16)	.	.	.	yes
C25	C26	C27	119.02(18)	.	.	.	no
C25	C26	C31	120.97(17)	.	.	.	no
C27	C26	C31	119.96(17)	.	.	.	no
C26	C27	C28	121.55(19)	.	.	.	no
C27	C28	C29	119.9(2)	.	.	.	no
C28	C29	C30	120.5(2)	.	.	.	no
C25	C30	C29	119.85(18)	.	.	.	no
C25	C30	C34	121.54(18)	.	.	.	no
C29	C30	C34	118.44(18)	.	.	.	no
C26	C31	C32	113.8(2)	.	.	.	no
C26	C31	C33	109.86(18)	.	.	.	no
C32	C31	C33	109.68(19)	.	.	.	no
C30	C34	C35	112.4(2)	.	.	.	no

C30	C34	C36	110.75(19)	.	.	.	no
C35	C34	C36	110.17(19)	.	.	.	no
C38	C37	C42	119.2(2)	.	.	.	no
C38	C37	B4	121.0(2)	.	.	.	yes
C42	C37	B4	119.79(19)	.	.	.	yes
C37	C38	C39	119.3(2)	.	.	.	no
C37	C38	C46	121.1(2)	.	.	.	no
C39	C38	C46	119.6(2)	.	.	.	no
C38	C39	C40	121.2(2)	.	.	.	no
C39	C40	C41	120.2(2)	.	.	.	no
C40	C41	C42	120.9(3)	.	.	.	no
C37	C42	C41	119.2(2)	.	.	.	no
C37	C42	C43	121.81(19)	.	.	.	no
C41	C42	C43	119.0(2)	.	.	.	no
C42	C43	C44	112.97(19)	.	.	.	no
C42	C43	C45	110.9(2)	.	.	.	no
C44	C43	C45	110.2(2)	.	.	.	no
C38	C46	C47	113.3(2)	.	.	.	no
C38	C46	C48	109.8(3)	.	.	.	no
C47	C46	C48	110.0(3)	.	.	.	no
A12	C49	C50	108.86(17)	.	.	.	yes
A12	C49	C51	110.02(16)	.	.	.	yes
A12	C49	C52	113.67(15)	.	.	.	yes
C50	C49	C51	107.90(19)	.	.	.	no
C50	C49	C52	109.3(2)	.	.	.	no
C51	C49	C52	106.9(2)	.	.	.	no
A12	C53	C54	114.50(16)	.	.	.	yes
A12	C53	C55	105.74(16)	.	.	.	yes
A12	C53	C56	112.52(17)	.	.	.	yes
C54	C53	C55	106.8(2)	.	.	.	no
C54	C53	C56	109.9(2)	.	.	.	no
C55	C53	C56	106.8(2)	.	.	.	no
A13	C57	C58	110.96(16)	.	.	.	yes
A13	C57	C59	113.73(15)	.	.	.	yes
A13	C57	C60	107.38(15)	.	.	.	yes
C58	C57	C59	108.79(19)	.	.	.	no
C58	C57	C60	107.5(2)	.	.	.	no
C59	C57	C60	108.3(2)	.	.	.	no
A14	C61	C62	106.38(15)	.	.	.	yes
A14	C61	C63	110.04(18)	.	.	.	yes
A14	C61	C64	116.05(18)	.	.	.	yes
C62	C61	C63	109.3(2)	.	.	.	no
C62	C61	C64	108.5(2)	.	.	.	no
C63	C61	C64	106.5(2)	.	.	.	no
C2	C3	H3	119.53	.	.	.	no
C4	C3	H3	119.49	.	.	.	no
C3	C4	H4	119.85	.	.	.	no
C5	C4	H4	119.79	.	.	.	no
C4	C5	H5	119.63	.	.	.	no
C6	C5	H5	119.70	.	.	.	no
C2	C7	H7	107.50	.	.	.	no
C8	C7	H7	107.53	.	.	.	no
C9	C7	H7	107.52	.	.	.	no
C7	C8	H8	109.50	.	.	.	no
C7	C8	H8'	109.47	.	.	.	no
C7	C8	H8"	109.46	.	.	.	no
H8	C8	H8'	109.50	.	.	.	no
H8	C8	H8"	109.47	.	.	.	no
H8'	C8	H8"	109.43	.	.	.	no
C7	C9	H9'	109.47	.	.	.	no
C7	C9	H9"	109.48	.	.	.	no
H9	C9	H9'	109.47	.	.	.	no
H9	C9	H9"	109.46	.	.	.	no
H9'	C9	H9"	109.49	.	.	.	no

C7	C9	H9	109.46	.	.	.	no
C11	C10	H10	106.95	.	.	.	no
C12	C10	H10	106.92	.	.	.	no
C6	C10	H10	106.93	.	.	.	no
C10	C11	H11'	109.48	.	.	.	no
C10	C11	H11"	109.49	.	.	.	no
H11	C11	H11'	109.45	.	.	.	no
H11	C11	H11"	109.47	.	.	.	no
H11'	C11	H11"	109.44	.	.	.	no
C10	C11	H11	109.50	.	.	.	no
C10	C12	H12	109.47	.	.	.	no
C10	C12	H12'	109.47	.	.	.	no
C10	C12	H12"	109.45	.	.	.	no
H12	C12	H12'	109.50	.	.	.	no
H12	C12	H12"	109.47	.	.	.	no
H12'	C12	H12"	109.47	.	.	.	no
C14	C15	H15	119.66	.	.	.	no
C16	C15	H15	119.67	.	.	.	no
C15	C16	H16	119.88	.	.	.	no
C17	C16	H16	119.87	.	.	.	no
C16	C17	H17	119.30	.	.	.	no
C18	C17	H17	119.29	.	.	.	no
C14	C19	H19	107.47	.	.	.	no
C20	C19	H19	107.47	.	.	.	no
C21	C19	H19	107.48	.	.	.	no
C19	C20	H20	109.47	.	.	.	no
H20	C20	H20'	109.48	.	.	.	no
H20	C20	H20"	109.47	.	.	.	no
H20'	C20	H20"	109.46	.	.	.	no
C19	C20	H20"	109.47	.	.	.	no
C19	C20	H20'	109.47	.	.	.	no
C19	C21	H21'	109.52	.	.	.	no
C19	C21	H21	109.50	.	.	.	no
H21	C21	H21"	109.42	.	.	.	no
C19	C21	H21"	109.45	.	.	.	no
H21	C21	H21'	109.50	.	.	.	no
H21'	C21	H21"	109.44	.	.	.	no
C23	C22	H22	107.69	.	.	.	no
C24	C22	H22	107.68	.	.	.	no
C18	C22	H22	107.68	.	.	.	no
C22	C23	H23"	109.46	.	.	.	no
C22	C23	H23	109.49	.	.	.	no
C22	C23	H23'	109.49	.	.	.	no
H23	C23	H23'	109.49	.	.	.	no
H23	C23	H23"	109.45	.	.	.	no
H23'	C23	H23"	109.45	.	.	.	no
C22	C24	H24	109.47	.	.	.	no
C22	C24	H24'	109.47	.	.	.	no
C22	C24	H24"	109.49	.	.	.	no
H24	C24	H24'	109.45	.	.	.	no
H24	C24	H24"	109.47	.	.	.	no
H24'	C24	H24"	109.48	.	.	.	no
C26	C27	H27	119.23	.	.	.	no
C28	C27	H27	119.23	.	.	.	no
C27	C28	H28	120.04	.	.	.	no
C29	C28	H28	120.05	.	.	.	no
C28	C29	H29	119.72	.	.	.	no
C30	C29	H29	119.74	.	.	.	no
C32	C31	H31	107.77	.	.	.	no
C33	C31	H31	107.79	.	.	.	no
C26	C31	H31	107.78	.	.	.	no
C31	C32	H32'	109.46	.	.	.	no
C31	C32	H32"	109.42	.	.	.	no
C31	C32	H32	109.47	.	.	.	no

H32	C32	H32"	109.47	.	.	.	no
H32'	C32	H32"	109.48	.	.	.	no
H32	C32	H32'	109.53	.	.	.	no
C31	C33	H33'	109.48	.	.	.	no
C31	C33	H33"	109.47	.	.	.	no
H33	C33	H33'	109.48	.	.	.	no
H33	C33	H33"	109.47	.	.	.	no
H33'	C33	H33"	109.46	.	.	.	no
C31	C33	H33	109.47	.	.	.	no
C30	C34	H34	107.78	.	.	.	no
C35	C34	H34	107.78	.	.	.	no
C36	C34	H34	107.79	.	.	.	no
C34	C35	H35	109.49	.	.	.	no
C34	C35	H35'	109.50	.	.	.	no
C34	C35	H35"	109.53	.	.	.	no
H35	C35	H35'	109.40	.	.	.	no
H35	C35	H35"	109.43	.	.	.	no
H35'	C35	H35"	109.47	.	.	.	no
C34	C36	H36	109.47	.	.	.	no
C34	C36	H36'	109.47	.	.	.	no
C34	C36	H36"	109.48	.	.	.	no
H36	C36	H36'	109.47	.	.	.	no
H36	C36	H36"	109.47	.	.	.	no
H36'	C36	H36"	109.47	.	.	.	no
C38	C39	H39	119.39	.	.	.	no
C40	C39	H39	119.43	.	.	.	no
C39	C40	H40	119.90	.	.	.	no
C41	C40	H40	119.89	.	.	.	no
C42	C41	H41	119.57	.	.	.	no
C40	C41	H41	119.50	.	.	.	no
C45	C43	H43	107.50	.	.	.	no
C44	C43	H43	107.50	.	.	.	no
C42	C43	H43	107.51	.	.	.	no
C43	C44	H44	109.47	.	.	.	no
C43	C44	H44'	109.52	.	.	.	no
C43	C44	H44"	109.48	.	.	.	no
H44'	C44	H44"	109.46	.	.	.	no
H44	C44	H44'	109.48	.	.	.	no
H44	C44	H44"	109.41	.	.	.	no
C43	C45	H45	109.47	.	.	.	no
C43	C45	H45'	109.47	.	.	.	no
C43	C45	H45"	109.48	.	.	.	no
H45	C45	H45'	109.45	.	.	.	no
H45	C45	H45"	109.47	.	.	.	no
H45'	C45	H45"	109.48	.	.	.	no
C38	C46	H46	107.86	.	.	.	no
C47	C46	H46	107.82	.	.	.	no
C48	C46	H46	107.86	.	.	.	no
C46	C47	H47	109.49	.	.	.	no
C46	C47	H47'	109.46	.	.	.	no
C46	C47	H47"	109.47	.	.	.	no
H47	C47	H47'	109.45	.	.	.	no
H47	C47	H47"	109.50	.	.	.	no
H47'	C47	H47"	109.46	.	.	.	no
C46	C48	H48	109.49	.	.	.	no
C46	C48	H48'	109.54	.	.	.	no
C46	C48	H48"	109.46	.	.	.	no
H48	C48	H48'	109.47	.	.	.	no
H48'	C48	H48"	109.44	.	.	.	no
H48	C48	H48"	109.43	.	.	.	no
C49	C50	H50'	109.48	.	.	.	no
C49	C50	H50"	109.48	.	.	.	no
H50	C50	H50'	109.47	.	.	.	no
H50	C50	H50"	109.45	.	.	.	no

H50'	C50	H50"	109.49	.	.	.	no
C49	C50	H50	109.45	.	.	.	no
C49	C51	H51	109.48	.	.	.	no
C49	C51	H51"	109.46	.	.	.	no
H51	C51	H51'	109.49	.	.	.	no
H51	C51	H51"	109.43	.	.	.	no
H51'	C51	H51"	109.46	.	.	.	no
C49	C51	H51'	109.50	.	.	.	no
C49	C52	H52	109.52	.	.	.	no
C49	C52	H52'	109.47	.	.	.	no
C49	C52	H52"	109.48	.	.	.	no
H52	C52	H52'	109.47	.	.	.	no
H52	C52	H52"	109.48	.	.	.	no
H52'	C52	H52"	109.41	.	.	.	no
C53	C54	H54	109.44	.	.	.	no
C53	C54	H54'	109.47	.	.	.	no
C53	C54	H54"	109.48	.	.	.	no
H54	C54	H54'	109.45	.	.	.	no
H54	C54	H54"	109.47	.	.	.	no
H54'	C54	H54"	109.51	.	.	.	no
C53	C55	H55	109.45	.	.	.	no
C53	C55	H55'	109.55	.	.	.	no
C53	C55	H55"	109.49	.	.	.	no
H55	C55	H55'	109.46	.	.	.	no
H55	C55	H55"	109.37	.	.	.	no
H55'	C55	H55"	109.51	.	.	.	no
C53	C56	H56"	109.48	.	.	.	no
H56	C56	H56'	109.47	.	.	.	no
H56	C56	H56"	109.44	.	.	.	no
H56'	C56	H56"	109.43	.	.	.	no
C53	C56	H56'	109.51	.	.	.	no
C53	C56	H56	109.51	.	.	.	no
C57	C58	H58"	109.41	.	.	.	no
C57	C58	H58	109.40	.	.	.	no
C57	C58	H58'	109.45	.	.	.	no
H58'	C58	H58"	109.55	.	.	.	no
H58	C58	H58'	109.54	.	.	.	no
H58	C58	H58"	109.48	.	.	.	no
C57	C59	H59	109.47	.	.	.	no
H59	C59	H59'	109.49	.	.	.	no
C57	C59	H59'	109.46	.	.	.	no
C57	C59	H59"	109.45	.	.	.	no
H59	C59	H59"	109.49	.	.	.	no
H59'	C59	H59"	109.47	.	.	.	no
C57	C60	H60	109.48	.	.	.	no
C57	C60	H60'	109.50	.	.	.	no
C57	C60	H60"	109.44	.	.	.	no
H60	C60	H60'	109.52	.	.	.	no
H60	C60	H60"	109.43	.	.	.	no
H60'	C60	H60"	109.46	.	.	.	no
C61	C62	H62	109.49	.	.	.	no
C61	C62	H62'	109.48	.	.	.	no
C61	C62	H62"	109.46	.	.	.	no
H62	C62	H62'	109.48	.	.	.	no
H62	C62	H62"	109.47	.	.	.	no
H62'	C62	H62"	109.45	.	.	.	no
C61	C63	H63	109.43	.	.	.	no
C61	C63	H63"	109.45	.	.	.	no
H63	C63	H63'	109.50	.	.	.	no
H63	C63	H63"	109.53	.	.	.	no
H63'	C63	H63"	109.49	.	.	.	no
C61	C63	H63'	109.42	.	.	.	no
C61	C64	H64	109.48	.	.	.	no
C61	C64	H64"	109.50	.	.	.	no

H64	C64	H64'	109.42	.	.	.	no
C61	C64	H64'	109.46	.	.	.	no
H64'	C64	H64"	109.48	.	.	.	no
H64	C64	H64"	109.48	.	.	.	no
C66	C65	C70	118.0(6)	.	.	.	no
C65	C66	C67	116.9(6)	.	.	.	no
C66	C67	C68	119.9(6)	.	.	.	no
C67	C68	C69	123.2(7)	.	.	.	no
C68	C69	C70	120.2(7)	.	.	.	no
C65	C70	C69	121.7(6)	.	.	.	no
C66	C65	H65	121.02	.	.	.	no
C70	C65	H65	120.96	.	.	.	no
C65	C66	H66	121.49	.	.	.	no
C67	C66	H66	121.56	.	.	.	no
C66	C67	H67	120.08	.	.	.	no
C68	C67	H67	120.05	.	.	.	no
C67	C68	H68	118.43	.	.	.	no
C69	C68	H68	118.40	.	.	.	no
C68	C69	H69	119.85	.	.	.	no
C70	C69	H69	119.94	.	.	.	no
C65	C70	H70	119.19	.	.	.	no
C69	C70	H70	119.06	.	.	.	no
C72B	C71B	C76B	120.0(5)	.	.	.	no
C71B	C72B	C73B	120.0(7)	.	.	.	no
C72B	C73B	C74B	120.0(7)	.	.	.	no
C73B	C74B	C75B	120.0(5)	.	.	.	no
C74B	C75B	C76B	120.0(6)	.	.	.	no
C71B	C76B	C75B	120.0(6)	.	.	.	no
C76B	C71B	H71B	119.98	.	.	.	no
C72B	C71B	H71B	120.02	.	.	.	no
C71B	C72B	H72B	119.95	.	.	.	no
C73B	C72B	H72B	120.03	.	.	.	no
C74B	C73B	H73B	120.03	.	.	.	no
C72B	C73B	H73B	119.97	.	.	.	no
C73B	C74B	H74B	120.04	.	.	.	no
C75B	C74B	H74B	119.97	.	.	.	no
C74B	C75B	H75B	119.98	.	.	.	no
C76B	C75B	H75B	120.06	.	.	.	no
C71B	C76B	H76B	120.03	.	.	.	no
C75B	C76B	H76B	119.94	.	.	.	no
C78	C77	C79	120.4(3)	.	.	.	no
C77	C78	C79	119.5(3)	.	.	2_566	no
C77	C79	C78	120.1(3)	.	.	2_566	no
C78	C77	H77	119.79	.	.	.	no
C79	C77	H77	119.78	.	.	.	no
C77	C78	H78	120.25	.	.	.	no
C79	C78	H78	120.29	2_566	.	.	no
C77	C79	H79	119.92	.	.	.	no
C78	C79	H79	119.96	2_566	.	.	no
C72A	C71A	C76A	119.9(17)	.	.	.	no
C71A	C72A	C73A	120.1(17)	.	.	.	no
C72A	C73A	C74A	120.0(17)	.	.	.	no
C73A	C74A	C75A	120.0(16)	.	.	.	no
C74A	C75A	C76A	120.0(18)	.	.	.	no
C71A	C76A	C75A	120.0(17)	.	.	.	no
C72A	C71A	H71	120.09	.	.	.	no
C76A	C71A	H71	120.02	.	.	.	no
C71A	C72A	H72	119.90	.	.	.	no
C73A	C72A	H72	120.02	.	.	.	no
C74A	C73A	H73	119.92	.	.	.	no
C72A	C73A	H73	120.05	.	.	.	no
C75A	C74A	H74	120.02	.	.	.	no
C73A	C74A	H74	120.01	.	.	.	no
C74A	C75A	H75	120.07	.	.	.	no

C76A	C75A	H75	119.92	.	.	.	no
C71A	C76A	H76	119.95	.	.	.	no
C75A	C76A	H76	120.03	.	.	.	no
Al1	B1	O1	51.83(9)	.	.	.	yes
Al1	B1	O2	54.10(9)	.	.	.	yes
Al1	B1	C1	173.62(15)	.	.	.	yes
O1	B1	O2	105.75(17)	.	.	.	yes
O1	B1	C1	133.03(19)	.	.	.	yes
O2	B1	C1	121.22(17)	.	.	.	yes
O4	B2	C13	118.92(15)	.	.	.	yes
O3	B2	C13	124.17(17)	.	.	.	yes
O3	B2	O4	116.91(16)	.	.	.	yes
O5	B3	C25	118.94(18)	.	.	.	yes
O6	B3	C25	123.47(18)	.	.	.	yes
O5	B3	O6	117.59(17)	.	.	.	yes
O8	B4	C37	124.0(2)	.	.	.	yes
O7	B4	O8	117.19(18)	.	.	.	yes
O7	B4	C37	118.74(18)	.	.	.	yes

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_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

O1	Al1	Al4	O4	125.93(10)	.	.	.	.	no
O1	Al1	Al4	O5	-12.23(10)	.	.	.	.	no
O1	Al1	Al4	O8	-120.79(10)	.	.	.	.	no
O2	Al1	Al4	O4	-28.91(8)	.	.	.	.	no
O2	Al1	Al4	O5	-167.06(9)	.	.	.	.	no
O2	Al1	Al4	O8	84.38(8)	.	.	.	.	no
O4	Al1	Al4	O5	-138.16(8)	.	.	.	.	no
O4	Al1	Al4	O8	113.28(7)	.	.	.	.	no
O5	Al1	Al4	O4	138.16(8)	.	.	.	.	no
O5	Al1	Al4	O8	-108.56(8)	.	.	.	.	no
O7	Al1	Al4	O4	-100.38(7)	.	.	.	.	no
O7	Al1	Al4	O5	121.47(7)	.	.	.	.	no
O7	Al1	Al4	O8	12.91(7)	.	.	.	.	no
Al4	Al1	O1	Al2	0.25(14)	.	.	.	.	no
Al4	Al1	O1	B1	-166.20(10)	.	.	.	.	no
O2	Al1	O1	Al2	163.02(9)	.	.	.	.	no
O2	Al1	O1	B1	-3.43(10)	.	.	.	.	no
O4	Al1	O1	Al2	86.89(12)	.	.	.	.	no
O4	Al1	O1	B1	-79.57(14)	.	.	.	.	no
O5	Al1	O1	Al2	-8.48(9)	.	.	.	.	no
O5	Al1	O1	B1	-174.93(10)	.	.	.	.	no
O7	Al1	O1	Al2	-126.45(8)	.	.	.	.	no
O7	Al1	O1	B1	67.10(11)	.	.	.	.	no
B1	Al1	O1	Al2	166.45(15)	.	.	.	.	no
Al4	Al1	O2	Al3	-48.83(8)	.	.	.	.	no
Al4	Al1	O2	B1	169.57(9)	.	.	.	.	no
O1	Al1	O2	Al3	145.06(6)	.	.	.	.	no
O1	Al1	O2	B1	3.45(10)	.	.	.	.	no
O4	Al1	O2	Al3	-68.85(6)	.	.	.	.	no
O4	Al1	O2	B1	149.54(10)	.	.	.	.	no
O7	Al1	O2	Al3	24.02(6)	.	.	.	.	no
O7	Al1	O2	B1	-117.59(11)	.	.	.	.	no
B1	Al1	O2	Al3	141.61(12)	.	.	.	.	no
Al4	Al1	O4	B2	-141.41(16)	.	.	.	.	no

O1	A11	O4	A14	-130.38(9)	.	.	.	.	no
O1	A11	O4	B2	88.21(16)	.	.	.	.	no
O2	A11	O4	A14	161.18(5)	.	.	.	.	no
O2	A11	O4	B2	19.77(14)	.	.	.	.	no
O5	A11	O4	A14	-27.97(6)	.	.	.	.	no
O5	A11	O4	B2	-169.38(14)	.	.	.	.	no
O7	A11	O4	A14	79.29(6)	.	.	.	.	no
O7	A11	O4	B2	-62.12(14)	.	.	.	.	no
B1	A11	O4	A14	-176.97(7)	.	.	.	.	no
B1	A11	O4	B2	41.62(17)	.	.	.	.	no
A14	A11	O5	B3	-158.29(16)	.	.	.	.	no
O1	A11	O5	A14	173.28(5)	.	.	.	.	no
O1	A11	O5	B3	14.98(15)	.	.	.	.	no
O4	A11	O5	A14	28.29(6)	.	.	.	.	no
O4	A11	O5	B3	-130.00(14)	.	.	.	.	no
O7	A11	O5	A14	-63.12(7)	.	.	.	.	no
O7	A11	O5	B3	138.58(14)	.	.	.	.	no
B1	A11	O5	A14	168.64(9)	.	.	.	.	no
B1	A11	O5	B3	10.35(19)	.	.	.	.	no
A14	A11	O7	A13	117.42(5)	.	.	.	.	no
A14	A11	O7	B4	-15.79(14)	.	.	.	.	no
O1	A11	O7	A13	-88.14(7)	.	.	.	.	no
O1	A11	O7	B4	138.65(14)	.	.	.	.	no
O2	A11	O7	A13	-23.18(6)	.	.	.	.	no
O2	A11	O7	B4	-156.39(15)	.	.	.	.	no
O4	A11	O7	A13	73.56(6)	.	.	.	.	no
O4	A11	O7	B4	-59.65(14)	.	.	.	.	no
O5	A11	O7	A13	155.91(6)	.	.	.	.	no
O5	A11	O7	B4	22.70(15)	.	.	.	.	no
B1	A11	O7	A13	-54.84(7)	.	.	.	.	no
B1	A11	O7	B4	171.95(14)	.	.	.	.	no
O1	A11	B1	O2	-174.43(16)	.	.	.	.	no
O2	A11	B1	O1	174.43(16)	.	.	.	.	no
O4	A11	B1	O1	135.36(10)	.	.	.	.	no
O4	A11	B1	O2	-39.07(13)	.	.	.	.	no
O5	A11	B1	O1	7.65(15)	.	.	.	.	no
O5	A11	B1	O2	-166.78(10)	.	.	.	.	no
O7	A11	B1	O1	-123.16(10)	.	.	.	.	no
O7	A11	B1	O2	62.41(10)	.	.	.	.	no
O6	A12	O1	A11	-2.09(9)	.	.	.	.	no
O6	A12	O1	B1	156.64(18)	.	.	.	.	no
C49	A12	O1	A11	-115.36(10)	.	.	.	.	no
C49	A12	O1	B1	43.4(2)	.	.	.	.	no
C53	A12	O1	A11	107.88(11)	.	.	.	.	no
C53	A12	O1	B1	-93.38(19)	.	.	.	.	no
O1	A12	O6	B3	19.7(3)	.	.	.	.	no
C49	A12	O6	B3	129.3(3)	.	.	.	.	no
C53	A12	O6	B3	-97.8(3)	.	.	.	.	no
O1	A12	C49	C50	53.91(16)	.	.	.	.	no
O1	A12	C49	C51	171.95(15)	.	.	.	.	no
O1	A12	C49	C52	-68.15(19)	.	.	.	.	no
O6	A12	C49	C50	-47.71(17)	.	.	.	.	no
O6	A12	C49	C51	70.34(18)	.	.	.	.	no
O6	A12	C49	C52	-169.77(16)	.	.	.	.	no
C53	A12	C49	C50	-172.46(15)	.	.	.	.	no
C53	A12	C49	C51	-54.42(19)	.	.	.	.	no
C53	A12	C49	C52	65.5(2)	.	.	.	.	no
O1	A12	C53	C54	91.44(19)	.	.	.	.	no
O1	A12	C53	C55	-151.21(16)	.	.	.	.	no
O1	A12	C53	C56	-35.02(19)	.	.	.	.	no
O6	A12	C53	C54	-165.60(17)	.	.	.	.	no
O6	A12	C53	C55	-48.25(19)	.	.	.	.	no
O6	A12	C53	C56	67.94(18)	.	.	.	.	no
C49	A12	C53	C54	-38.6(2)	.	.	.	.	no

C49	A12	C53	C55	78.72(19)	.	.	.	.	no
C49	A12	C53	C56	-165.09(16)	.	.	.	.	no
O3	A13	O2	A11	78.59(6)	.	.	.	.	no
O3	A13	O2	B1	171.85(19)	.	.	.	.	no
O7	A13	O2	A11	-23.40(5)	.	.	.	.	no
O7	A13	O2	B1	69.86(19)	.	.	.	.	no
C57	A13	O2	A11	-150.83(9)	.	.	.	.	no
C57	A13	O2	B1	-57.6(2)	.	.	.	.	no
O2	A13	O3	B2	-38.98(17)	.	.	.	.	no
O7	A13	O3	B2	45.57(17)	.	.	.	.	no
C57	A13	O3	B2	-173.15(16)	.	.	.	.	no
O2	A13	O7	A11	24.40(6)	.	.	.	.	no
O2	A13	O7	B4	155.20(14)	.	.	.	.	no
O3	A13	O7	A11	-71.96(7)	.	.	.	.	no
O3	A13	O7	B4	58.85(15)	.	.	.	.	no
C57	A13	O7	A11	150.45(10)	.	.	.	.	no
C57	A13	O7	B4	-78.75(17)	.	.	.	.	no
O2	A13	C57	C58	-7.3(2)	.	.	.	.	no
O2	A13	C57	C59	115.76(18)	.	.	.	.	no
O2	A13	C57	C60	-124.50(16)	.	.	.	.	no
O3	A13	C57	C58	114.47(16)	.	.	.	.	no
O3	A13	C57	C59	-122.49(17)	.	.	.	.	no
O3	A13	C57	C60	-2.7(2)	.	.	.	.	no
O7	A13	C57	C58	-113.52(16)	.	.	.	.	no
O7	A13	C57	C59	9.5(2)	.	.	.	.	no
O7	A13	C57	C60	129.26(15)	.	.	.	.	no
A11	A14	O4	B2	136.54(16)	.	.	.	.	no
O5	A14	O4	A11	27.53(5)	.	.	.	.	no
O5	A14	O4	B2	164.07(15)	.	.	.	.	no
O8	A14	O4	A11	-68.93(7)	.	.	.	.	no
O8	A14	O4	B2	67.61(15)	.	.	.	.	no
C61	A14	O4	A11	162.82(8)	.	.	.	.	no
C61	A14	O4	B2	-60.64(17)	.	.	.	.	no
A11	A14	O5	B3	156.16(18)	.	.	.	.	no
O4	A14	O5	A11	-28.28(5)	.	.	.	.	no
O4	A14	O5	B3	127.88(16)	.	.	.	.	no
O8	A14	O5	A11	72.30(7)	.	.	.	.	no
O8	A14	O5	B3	-131.53(16)	.	.	.	.	no
C61	A14	O5	A11	-153.20(10)	.	.	.	.	no
C61	A14	O5	B3	3.0(2)	.	.	.	.	no
A11	A14	O8	B4	-12.68(18)	.	.	.	.	no
O4	A14	O8	B4	28.40(19)	.	.	.	.	no
O5	A14	O8	B4	-53.55(19)	.	.	.	.	no
C61	A14	O8	B4	161.27(18)	.	.	.	.	no
O4	A14	C61	C62	56.70(18)	.	.	.	.	no
O4	A14	C61	C63	174.94(18)	.	.	.	.	no
O4	A14	C61	C64	-64.1(2)	.	.	.	.	no
O5	A14	C61	C62	164.88(13)	.	.	.	.	no
O5	A14	C61	C63	-76.9(2)	.	.	.	.	no
O5	A14	C61	C64	44.1(2)	.	.	.	.	no
O8	A14	C61	C62	-65.84(17)	.	.	.	.	no
O8	A14	C61	C63	52.4(2)	.	.	.	.	no
O8	A14	C61	C64	173.41(19)	.	.	.	.	no
A11	O1	B1	O2	4.69(14)	.	.	.	.	no
A11	O1	B1	C1	-174.6(2)	.	.	.	.	no
A12	O1	B1	A11	-162.95(18)	.	.	.	.	no
A12	O1	B1	O2	-158.26(12)	.	.	.	.	no
A12	O1	B1	C1	22.5(3)	.	.	.	.	no
A11	O2	B1	O1	-4.55(13)	.	.	.	.	no
A11	O2	B1	C1	174.80(17)	.	.	.	.	no
A13	O2	B1	A11	-94.12(17)	.	.	.	.	no
A13	O2	B1	O1	-98.67(19)	.	.	.	.	no
A13	O2	B1	C1	80.7(3)	.	.	.	.	no
A13	O3	B2	O4	-20.0(3)	.	.	.	.	no

A13	O3	B2	C13	159.32(15)	.	.	.	.	no
A11	O4	B2	O3	29.2(2)	.	.	.	.	no
A11	O4	B2	C13	-150.13(14)	.	.	.	.	no
A14	O4	B2	O3	-95.8(2)	.	.	.	.	no
A14	O4	B2	C13	84.8(2)	.	.	.	.	no
A11	O5	B3	O6	-6.9(2)	.	.	.	.	no
A11	O5	B3	C25	172.65(12)	.	.	.	.	no
A14	O5	B3	O6	-155.95(13)	.	.	.	.	no
A14	O5	B3	C25	23.6(3)	.	.	.	.	no
A12	O6	B3	O5	-16.8(4)	.	.	.	.	no
A12	O6	B3	C25	163.66(17)	.	.	.	.	no
A11	O7	B4	O8	12.6(2)	.	.	.	.	no
A11	O7	B4	C37	-169.19(14)	.	.	.	.	no
A13	O7	B4	O8	-105.75(18)	.	.	.	.	no
A13	O7	B4	C37	72.4(2)	.	.	.	.	no
A14	O8	B4	O7	4.8(3)	.	.	.	.	no
A14	O8	B4	C37	-173.31(15)	.	.	.	.	no
C6	C1	C2	C3	1.0(3)	.	.	.	.	no
C6	C1	C2	C7	-178.4(2)	.	.	.	.	no
B1	C1	C2	C3	-171.3(2)	.	.	.	.	no
B1	C1	C2	C7	9.4(3)	.	.	.	.	no
C2	C1	C6	C5	-1.9(3)	.	.	.	.	no
C2	C1	C6	C10	-179.4(2)	.	.	.	.	no
B1	C1	C6	C5	170.0(2)	.	.	.	.	no
B1	C1	C6	C10	-7.5(3)	.	.	.	.	no
C2	C1	B1	O1	-123.2(2)	.	.	.	.	no
C2	C1	B1	O2	57.7(3)	.	.	.	.	no
C6	C1	B1	O1	64.8(3)	.	.	.	.	no
C6	C1	B1	O2	-114.4(2)	.	.	.	.	no
C1	C2	C3	C4	0.5(4)	.	.	.	.	no
C7	C2	C3	C4	179.9(3)	.	.	.	.	no
C1	C2	C7	C8	-110.6(3)	.	.	.	.	no
C1	C2	C7	C9	124.6(2)	.	.	.	.	no
C3	C2	C7	C8	70.0(3)	.	.	.	.	no
C3	C2	C7	C9	-54.7(3)	.	.	.	.	no
C2	C3	C4	C5	-1.1(5)	.	.	.	.	no
C3	C4	C5	C6	0.1(4)	.	.	.	.	no
C4	C5	C6	C1	1.4(4)	.	.	.	.	no
C4	C5	C6	C10	178.9(2)	.	.	.	.	no
C1	C6	C10	C11	-158.0(2)	.	.	.	.	no
C1	C6	C10	C12	77.3(3)	.	.	.	.	no
C5	C6	C10	C11	24.6(3)	.	.	.	.	no
C5	C6	C10	C12	-100.2(3)	.	.	.	.	no
C18	C13	C14	C15	1.6(3)	.	.	.	.	no
C18	C13	C14	C19	-177.14(18)	.	.	.	.	no
B2	C13	C14	C15	-179.26(19)	.	.	.	.	no
B2	C13	C14	C19	2.0(3)	.	.	.	.	no
C14	C13	C18	C17	-1.6(3)	.	.	.	.	no
C14	C13	C18	C22	176.53(18)	.	.	.	.	no
B2	C13	C18	C17	179.25(19)	.	.	.	.	no
B2	C13	C18	C22	-2.6(3)	.	.	.	.	no
C14	C13	B2	O3	-124.8(2)	.	.	.	.	no
C14	C13	B2	O4	54.5(3)	.	.	.	.	no
C18	C13	B2	O3	54.3(3)	.	.	.	.	no
C18	C13	B2	O4	-126.3(2)	.	.	.	.	no
C13	C14	C15	C16	-0.4(3)	.	.	.	.	no
C19	C14	C15	C16	178.4(2)	.	.	.	.	no
C13	C14	C19	C20	130.1(2)	.	.	.	.	no
C13	C14	C19	C21	-105.5(2)	.	.	.	.	no
C15	C14	C19	C20	-48.7(3)	.	.	.	.	no
C15	C14	C19	C21	75.8(2)	.	.	.	.	no
C14	C15	C16	C17	-0.8(4)	.	.	.	.	no
C15	C16	C17	C18	0.8(4)	.	.	.	.	no
C16	C17	C18	C13	0.4(3)	.	.	.	.	no

C16	C17	C18	C22	-177.7(2)	.	.	.	.	no
C13	C18	C22	C23	-94.8(2)	.	.	.	.	no
C13	C18	C22	C24	141.4(2)	.	.	.	.	no
C17	C18	C22	C23	83.3(3)	.	.	.	.	no
C17	C18	C22	C24	-40.4(3)	.	.	.	.	no
C30	C25	C26	C27	-1.3(3)	.	.	.	.	no
C30	C25	C26	C31	176.2(2)	.	.	.	.	no
B3	C25	C26	C27	-176.6(2)	.	.	.	.	no
B3	C25	C26	C31	0.9(3)	.	.	.	.	no
C26	C25	C30	C29	0.6(3)	.	.	.	.	no
C26	C25	C30	C34	-174.6(2)	.	.	.	.	no
B3	C25	C30	C29	175.9(2)	.	.	.	.	no
B3	C25	C30	C34	0.7(3)	.	.	.	.	no
C26	C25	B3	O5	-111.9(2)	.	.	.	.	no
C26	C25	B3	O6	67.7(3)	.	.	.	.	no
C30	C25	B3	O5	72.8(3)	.	.	.	.	no
C30	C25	B3	O6	-107.6(2)	.	.	.	.	no
C25	C26	C27	C28	1.0(3)	.	.	.	.	no
C31	C26	C27	C28	-176.5(2)	.	.	.	.	no
C25	C26	C31	C32	142.3(2)	.	.	.	.	no
C25	C26	C31	C33	-94.3(2)	.	.	.	.	no
C27	C26	C31	C32	-40.3(3)	.	.	.	.	no
C27	C26	C31	C33	83.1(2)	.	.	.	.	no
C26	C27	C28	C29	-0.2(4)	.	.	.	.	no
C27	C28	C29	C30	-0.5(4)	.	.	.	.	no
C28	C29	C30	C25	0.3(4)	.	.	.	.	no
C28	C29	C30	C34	175.6(2)	.	.	.	.	no
C25	C30	C34	C35	-134.1(2)	.	.	.	.	no
C25	C30	C34	C36	102.2(2)	.	.	.	.	no
C29	C30	C34	C35	50.7(3)	.	.	.	.	no
C29	C30	C34	C36	-73.0(3)	.	.	.	.	no
C42	C37	C38	C39	-0.8(3)	.	.	.	.	no
C42	C37	C38	C46	-177.4(2)	.	.	.	.	no
B4	C37	C38	C39	178.6(2)	.	.	.	.	no
B4	C37	C38	C46	2.0(3)	.	.	.	.	no
C38	C37	C42	C41	0.1(3)	.	.	.	.	no
C38	C37	C42	C43	179.6(2)	.	.	.	.	no
B4	C37	C42	C41	-179.3(2)	.	.	.	.	no
B4	C37	C42	C43	0.2(3)	.	.	.	.	no
C38	C37	B4	O7	66.4(3)	.	.	.	.	no
C38	C37	B4	O8	-115.6(3)	.	.	.	.	no
C42	C37	B4	O7	-114.2(2)	.	.	.	.	no
C42	C37	B4	O8	63.8(3)	.	.	.	.	no
C37	C38	C39	C40	0.4(4)	.	.	.	.	no
C46	C38	C39	C40	177.1(2)	.	.	.	.	no
C37	C38	C46	C47	-152.4(3)	.	.	.	.	no
C37	C38	C46	C48	84.2(3)	.	.	.	.	no
C39	C38	C46	C47	31.0(4)	.	.	.	.	no
C39	C38	C46	C48	-92.4(3)	.	.	.	.	no
C38	C39	C40	C41	0.6(4)	.	.	.	.	no
C39	C40	C41	C42	-1.2(4)	.	.	.	.	no
C40	C41	C42	C37	0.9(4)	.	.	.	.	no
C40	C41	C42	C43	-178.6(2)	.	.	.	.	no
C37	C42	C43	C44	136.3(2)	.	.	.	.	no
C37	C42	C43	C45	-99.4(3)	.	.	.	.	no
C41	C42	C43	C44	-44.2(3)	.	.	.	.	no
C41	C42	C43	C45	80.1(3)	.	.	.	.	no
C70	C65	C66	C67	-0.3(8)	.	.	.	.	no
C66	C65	C70	C69	-0.9(9)	.	.	.	.	no
C65	C66	C67	C68	0.3(9)	.	.	.	.	no
C66	C67	C68	C69	0.9(10)	.	.	.	.	no
C67	C68	C69	C70	-2.1(12)	.	.	.	.	no
C68	C69	C70	C65	2.1(11)	.	.	.	.	no
C76B	C71B	C72B	C73B	0.0(14)	.	.	.	.	no

C72B	C71B	C76B	C75B	-0.1(13)	.	.	.	.	no
C71B	C72B	C73B	C74B	0.1(16)	.	.	.	.	no
C72B	C73B	C74B	C75B	0.0(16)	.	.	.	.	no
C73B	C74B	C75B	C76B	0.0(13)	.	.	.	.	no
C74B	C75B	C76B	C71B	0.1(13)	.	.	.	.	no
C79	C77	C78	C79	0.0(4)	.	.	.	2_566	no
C78	C77	C79	C78	0.0(4)	.	.	.	2_566	no
C77	C78	C79	C77	0.0(4)	.	.	2_566	2_566	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

Al4	C30	4.040(2)	.	.	.	no
Al1	H19	3.3093	.	.	.	no
Al2	H10	3.2525	.	.	.	no
Al3	H12	3.1383	.	.	.	no
Al3	H43	3.5238	.	.	.	no
Al3	H8"	3.5272	.	.	.	no
Al4	H21"	3.5077	.	.	.	no
O1	C10	3.412(3)	.	.	.	no
O2	C7	3.173(3)	.	.	.	no
O3	C22	3.161(3)	.	.	.	no
O3	C23	3.376(3)	.	.	.	no
O4	C19	3.133(2)	.	.	.	no
O5	C34	3.404(2)	.	.	.	no
O6	C31	3.285(2)	.	.	.	no
O6	C33	3.405(3)	.	.	.	no
O7	C46	3.299(3)	.	.	.	no
O8	C43	3.255(3)	.	.	.	no
O1	H10	2.7158	.	.	.	no
O2	H7	2.5708	.	.	.	no
O3	H22	2.5750	.	.	.	no
O3	H23"	2.7539	.	.	.	no
O4	H21"	2.8874	.	.	.	no
O4	H19	2.5067	.	.	.	no
O5	H34	2.6289	.	.	.	no
O6	H50'	2.8732	.	.	.	no
O6	H31	2.7828	.	.	.	no
O6	H33"	2.7303	.	.	.	no
O6	H55	2.6777	.	.	.	no
O7	H46	2.5209	.	.	.	no
O8	H43	2.6746	.	.	.	no
O8	H45"	2.8838	.	.	.	no
C7	O2	3.173(3)	.	.	.	no
C10	O1	3.412(3)	.	.	.	no
C12	B1	3.328(4)	.	.	.	no
C19	O4	3.133(2)	.	.	.	no
C22	O3	3.161(3)	.	.	.	no
C23	O3	3.376(3)	.	.	.	no
C30	Al4	4.040(2)	.	.	.	no
C31	O6	3.285(2)	.	.	.	no
C33	O6	3.405(3)	.	.	.	no
C34	O5	3.404(2)	.	.	.	no
C43	O8	3.255(3)	.	.	.	no
C46	O7	3.299(3)	.	.	.	no
C47	C75B	3.359(8)	.	.	.	no
C48	B4	3.492(5)	.	.	.	no
C75B	C47	3.359(8)	.	.	.	no
C1	H12	2.9937	.	.	.	no
C1	H52	2.7364	.	.	.	no

C2	H52	2.9130	.	.	no
C3	H9"	2.7977	.	.	no
C3	H8	2.8690	.	.	no
C5	H11	2.7559	.	.	no
C5	H11"	2.9254	.	.	no
C8	H3	3.0396	.	.	no
C9	H3	2.8233	.	.	no
C10	H54"	2.8288	.	.	no
C10	H56'	2.9026	.	.	no
C11	H54"	2.7633	.	.	no
C11	H5	2.5550	.	.	no
C12	H58	2.8690	.	.	no
C12	H59'	2.9913	.	.	no
C13	H65	3.0649	.	1_565	no
C13	H62"	2.9042	.	.	no
C15	H20"	2.7604	.	.	no
C15	H21	2.9046	.	.	no
C17	H24"	2.7774	.	.	no
C17	H24	3.0495	.	.	no
C17	H23	3.0029	.	.	no
C18	H62"	2.8423	.	.	no
C20	H15	2.7301	.	.	no
C21	H31	3.0847	.	.	no
C21	H15	3.0894	.	.	no
C23	H74B	3.0081	.	2_576	no
C24	H17	2.6606	.	.	no
C25	H64'	3.0935	.	.	no
C26	H64'	2.7471	.	.	no
C27	H33	3.0420	.	.	no
C27	H32"	2.8540	.	.	no
C27	H32	3.0010	.	.	no
C28	H16	2.9966	.	2_576	no
C29	H35	2.7088	.	.	no
C29	H36"	2.9128	.	.	no
C30	H63'	3.0024	.	.	no
C31	H64'	3.0514	.	.	no
C32	H64'	2.9751	.	.	no
C32	H27	2.6794	.	.	no
C33	H51'	2.9829	.	.	no
C35	H48	2.9084	.	.	no
C35	H29	2.7394	.	.	no
C36	H29	3.0996	.	.	no
C37	H59	2.9270	.	.	no
C37	H48	2.9898	.	.	no
C39	H47'	2.8700	.	.	no
C39	H47"	2.8033	.	.	no
C40	H68	3.0668	.	.	no
C41	H68	3.0584	.	.	no
C41	H44	2.7259	.	.	no
C41	H45	2.9814	.	.	no
C42	H59	2.9821	.	.	no
C44	H41	2.6929	.	.	no
C45	H52'	3.0156	.	2_576	no
C47	H39	2.5617	.	.	no
C47	H75B	2.6319	.	.	no
C47	H12'	2.8144	.	.	no
C48	H35'	2.9038	.	.	no
C50	H21'	3.0459	.	.	no
C51	H55'	3.0475	.	.	no
C52	H9	3.0839	.	.	no
C52	H45'	3.0429	.	1_655	no
C53	H10	3.0257	.	.	no
C54	H52'	3.0614	.	.	no
C54	H10	2.9338	.	.	no

C56	H10	2.9099	.	.	no
C59	H11	3.0738	.	2_675	no
C60	H73B	3.0622	.	2_576	no
C62	H24	2.9780	.	.	no
C63	H35"	3.0655	.	.	no
C64	H32	2.8369	.	.	no
C69	H71	3.0827	.	1_545	no
C72A	H69	3.0923	.	2_665	no
C73A	H58"	3.0148	.	2_675	no
C74B	H23'	3.0816	.	2_665	no
C75B	H47	2.8055	.	.	no
C75B	H47"	3.0538	.	.	no
B1	C12	3.328(4)	.	.	no
B4	C48	3.492(5)	.	.	no
B1	H12	2.7180	.	.	no
B1	H7	2.4449	.	.	no
B1	H10	2.7158	.	.	no
B2	H19	2.5144	.	.	no
B2	H22	2.5499	.	.	no
B3	H31	2.5090	.	.	no
B3	H34	2.5041	.	.	no
B4	H48	2.9657	.	.	no
B4	H46	2.6081	.	.	no
B4	H43	2.4856	.	.	no
H3	H9"	2.3040	.	.	no
H3	C9	2.8233	.	.	no
H3	H8	2.5332	.	.	no
H3	C8	3.0396	.	.	no
H5	H11"	2.5803	.	.	no
H5	H11	2.1498	.	.	no
H5	C11	2.5550	.	.	no
H7	B1	2.4449	.	.	no
H7	O2	2.5708	.	.	no
H7	H50"	2.4980	.	.	no
H8	H3	2.5332	.	.	no
H8	H71B	2.5595	.	2_675	no
H8	H9"	2.5873	.	.	no
H8	C3	2.8690	.	.	no
H8'	H20	2.4688	.	.	no
H8'	H9'	2.5084	.	.	no
H8"	A13	3.5272	.	.	no
H8"	H58'	2.5175	.	.	no
H9	C52	3.0839	.	.	no
H9	H52	2.5155	.	.	no
H9'	H8'	2.5084	.	.	no
H9'	H20'	2.5137	.	.	no
H9"	H3	2.3040	.	.	no
H9"	C3	2.7977	.	.	no
H9"	H8	2.5873	.	.	no
H9"	H36'	2.5999	.	2_675	no
H10	C56	2.9099	.	.	no
H10	O1	2.7158	.	.	no
H10	H56'	2.1219	.	.	no
H10	A12	3.2525	.	.	no
H10	C54	2.9338	.	.	no
H10	B1	2.7158	.	.	no
H10	H54"	2.1683	.	.	no
H10	C53	3.0257	.	.	no
H11	H59"	2.5778	.	2_675	no
H11	H5	2.1498	.	.	no
H11	C5	2.7559	.	.	no
H11	C59	3.0738	.	2_675	no
H11	H12"	2.5412	.	.	no
H11'	H12'	2.4080	.	.	no

H11"	H5	2.5803	.	.	no
H11"	H54"	2.3137	.	.	no
H11"	C5	2.9254	.	.	no
H12	B1	2.7180	.	.	no
H12	C1	2.9937	.	.	no
H12	A13	3.1383	.	.	no
H12	H58	2.5009	.	.	no
H12	H59'	2.5489	.	.	no
H12'	H11'	2.4080	.	.	no
H12'	C47	2.8144	.	.	no
H12'	H47	2.4209	.	.	no
H12'	H47'	2.5333	.	.	no
H12"	H11	2.5412	.	.	no
H12"	H58	2.4625	.	.	no
H15	H20"	2.2228	.	.	no
H15	C21	3.0894	.	.	no
H15	C20	2.7301	.	.	no
H16	C28	2.9966	.	2_576	no
H17	C24	2.6606	.	.	no
H17	H24"	2.1855	.	.	no
H19	A11	3.3093	.	.	no
H19	O4	2.5067	.	.	no
H19	B2	2.5144	.	.	no
H20	H8'	2.4688	.	.	no
H20'	H9'	2.5137	.	.	no
H20'	H21'	2.4869	.	.	no
H20"	H21	2.5481	.	.	no
H20"	C15	2.7604	.	.	no
H20"	H15	2.2228	.	.	no
H21	H20"	2.5481	.	.	no
H21	C15	2.9046	.	.	no
H21'	H50'	2.5263	.	.	no
H21'	C50	3.0459	.	.	no
H21'	H20'	2.4869	.	.	no
H21"	H31	2.5821	.	.	no
H21"	H64	2.4148	.	.	no
H21"	A14	3.5077	.	.	no
H21"	O4	2.8874	.	.	no
H22	H43	2.4469	.	.	no
H22	B2	2.5499	.	.	no
H22	O3	2.5750	.	.	no
H23	C17	3.0029	.	.	no
H23	H24"	2.5373	.	.	no
H23'	C74B	3.0816	.	1_465	no
H23'	H44"	2.4223	.	.	no
H23'	H24'	2.4983	.	.	no
H23'	H74B	2.5458	.	2_576	no
H23"	H70	2.5191	.	1_565	no
H23"	O3	2.7539	.	.	no
H24	C17	3.0495	.	.	no
H24	C62	2.9780	.	.	no
H24'	H23'	2.4983	.	.	no
H24'	H44"	2.5423	.	.	no
H24"	H17	2.1855	.	.	no
H24"	C17	2.7774	.	.	no
H24"	H23	2.5373	.	.	no
H27	H36"	2.5980	.	2_666	no
H27	H32"	2.2690	.	.	no
H27	C32	2.6794	.	.	no
H29	H35	2.1699	.	.	no
H29	C35	2.7394	.	.	no
H29	H33	2.4761	.	2_666	no
H29	C36	3.0996	.	.	no
H31	B3	2.5090	.	.	no

H31	C21	3.0847	.	.	no
H31	O6	2.7828	.	.	no
H31	H21"	2.5821	.	.	no
H32	C64	2.8369	.	.	no
H32	C27	3.0010	.	.	no
H32	H64'	2.2002	.	.	no
H32'	H33'	2.5649	.	.	no
H32'	H50	2.5093	.	1_545	no
H32"	C27	2.8540	.	.	no
H32"	H27	2.2690	.	.	no
H32"	H33	2.4590	.	.	no
H33	C27	3.0420	.	.	no
H33	H32"	2.4590	.	.	no
H33	H29	2.4761	.	2_666	no
H33'	H32'	2.5649	.	.	no
H33"	H51'	2.3303	.	.	no
H33"	O6	2.7303	.	.	no
H34	O5	2.6289	.	.	no
H34	B3	2.5041	.	.	no
H35	C29	2.7088	.	.	no
H35	H29	2.1699	.	.	no
H35	H36"	2.5506	.	.	no
H35'	H36'	2.4712	.	.	no
H35'	C48	2.9038	.	.	no
H35'	H48	2.2915	.	.	no
H35"	H67	2.5781	.	.	no
H35"	C63	3.0655	.	.	no
H35"	H63"	2.5689	.	.	no
H36	H55	2.3863	.	.	no
H36'	H9"	2.5999	.	1_545	no
H36'	H35'	2.4712	.	.	no
H36"	H35	2.5506	.	.	no
H36"	C29	2.9128	.	.	no
H36"	H27	2.5980	.	2_666	no
H39	H47'	2.5508	.	.	no
H39	H47"	2.1959	.	.	no
H39	C47	2.5617	.	.	no
H41	C44	2.6929	.	.	no
H41	H44	2.1619	.	.	no
H43	A13	3.5238	.	.	no
H43	H22	2.4469	.	.	no
H43	O8	2.6746	.	.	no
H43	B4	2.4856	.	.	no
H44	H41	2.1619	.	.	no
H44	C41	2.7259	.	.	no
H44	H45	2.5370	.	.	no
H44'	H60"	2.3006	.	.	no
H44"	H24'	2.5423	.	.	no
H44"	H45'	2.4543	.	.	no
H44"	H23'	2.4223	.	.	no
H45	C41	2.9814	.	.	no
H45	H44	2.5370	.	.	no
H45'	H52'	2.4850	.	2_576	no
H45'	C52	3.0429	.	1_455	no
H45'	H44"	2.4543	.	.	no
H45"	O8	2.8838	.	.	no
H46	B4	2.6081	.	.	no
H46	O7	2.5209	.	.	no
H47	H75B	2.2125	.	.	no
H47	H75	2.5669	.	.	no
H47	H48'	2.5376	.	.	no
H47	C75B	2.8055	.	.	no
H47	H12'	2.4209	.	.	no
H47'	H12'	2.5333	.	.	no

H47'	C39	2.8700	.	.	no
H47'	H39	2.5508	.	.	no
H47"	C39	2.8033	.	.	no
H47"	H76	2.4995	.	1_545	no
H47"	H39	2.1959	.	.	no
H47"	H48"	2.4311	.	.	no
H47"	H75B	2.2251	.	.	no
H47"	C75B	3.0538	.	.	no
H48	C35	2.9084	.	.	no
H48	H35'	2.2915	.	.	no
H48	C37	2.9898	.	.	no
H48	B4	2.9657	.	.	no
H48'	H47	2.5376	.	.	no
H48"	H47"	2.4311	.	.	no
H50	H32'	2.5093	.	1_545	no
H50	H52"	2.4799	.	.	no
H50	H51"	2.4427	.	.	no
H50'	O6	2.8732	.	.	no
H50'	H21'	2.5263	.	.	no
H50'	H51'	2.4996	.	.	no
H50"	H7	2.4980	.	.	no
H50"	H52	2.5137	.	.	no
H51	H55'	2.4252	.	.	no
H51	H52'	2.4827	.	.	no
H51'	H50'	2.4996	.	.	no
H51'	H33"	2.3303	.	.	no
H51'	C33	2.9829	.	.	no
H51"	H52"	2.4072	.	.	no
H51"	H50	2.4427	.	.	no
H52	H50"	2.5137	.	.	no
H52	H9	2.5155	.	.	no
H52	C1	2.7364	.	.	no
H52	C2	2.9130	.	.	no
H52'	H45'	2.4850	.	1_655	no
H52'	H54'	2.5263	.	.	no
H52'	H51	2.4827	.	.	no
H52'	C45	3.0156	.	1_655	no
H52'	C54	3.0614	.	.	no
H52"	H51"	2.4072	.	.	no
H52"	H50	2.4799	.	.	no
H54	H55"	2.4875	.	.	no
H54	H56	2.4302	.	.	no
H54'	H52'	2.5263	.	.	no
H54'	H55'	2.4194	.	.	no
H54"	H11"	2.3137	.	.	no
H54"	C11	2.7633	.	.	no
H54"	H10	2.1683	.	.	no
H54"	C10	2.8288	.	.	no
H55	O6	2.6777	.	.	no
H55	H36	2.3863	.	.	no
H55	H56"	2.4735	.	.	no
H55'	C51	3.0475	.	.	no
H55'	H51	2.4252	.	.	no
H55'	H54'	2.4194	.	.	no
H55"	H56	2.4155	.	.	no
H55"	H54	2.4875	.	.	no
H56	H54	2.4302	.	.	no
H56	H55"	2.4155	.	.	no
H56'	C10	2.9026	.	.	no
H56'	H10	2.1219	.	.	no
H56"	H55	2.4735	.	.	no
H58	H59'	2.5044	.	.	no
H58	H12"	2.4625	.	.	no
H58	H12	2.5009	.	.	no

H58	C12	2.8690	.	.	no
H58'	H60'	2.4865	.	.	no
H58'	H8"	2.5175	.	.	no
H58"	H60	2.4524	.	.	no
H58"	H59"	2.4924	.	.	no
H58"	C73A	3.0148	.	2_675	no
H59	C42	2.9821	.	.	no
H59	C37	2.9270	.	.	no
H59	H60"	2.5273	.	.	no
H59'	H12	2.5489	.	.	no
H59'	C12	2.9913	.	.	no
H59'	H58	2.5044	.	.	no
H59"	H11	2.5778	.	2_675	no
H59"	H60	2.4242	.	.	no
H59"	H58"	2.4924	.	.	no
H60	H58"	2.4524	.	.	no
H60	H59"	2.4242	.	.	no
H60'	H58'	2.4865	.	.	no
H60'	H70	2.5250	.	1_565	no
H60"	H44'	2.3006	.	.	no
H60"	H59	2.5273	.	.	no
H62	H64"	2.4714	.	.	no
H62	H63	2.4007	.	.	no
H62'	H63"	2.5636	.	.	no
H62"	H64	2.4605	.	.	no
H62"	C13	2.9042	.	.	no
H62"	C18	2.8423	.	.	no
H63	H64"	2.4192	.	.	no
H63	H62	2.4007	.	.	no
H63'	C30	3.0024	.	.	no
H63'	H64'	2.4235	.	.	no
H63"	H35"	2.5689	.	.	no
H63"	H62'	2.5636	.	.	no
H64	H62"	2.4605	.	.	no
H64	H21"	2.4148	.	.	no
H64'	C32	2.9751	.	.	no
H64'	C31	3.0514	.	.	no
H64'	C25	3.0935	.	.	no
H64'	C26	2.7471	.	.	no
H64'	H32	2.2002	.	.	no
H64'	H63'	2.4235	.	.	no
H64"	H62	2.4714	.	.	no
H64"	H63	2.4192	.	.	no
H65	C13	3.0649	.	1_545	no
H67	H35"	2.5781	.	.	no
H68	C40	3.0668	.	.	no
H68	C41	3.0584	.	.	no
H69	H72B	2.5156	.	2_665	no
H69	H73	2.5268	.	2_665	no
H69	H72	2.4284	.	1_545	no
H69	C72A	3.0923	.	2_665	no
H70	H60'	2.5250	.	1_545	no
H70	H23"	2.5191	.	1_545	no
H71	C69	3.0827	.	2_665	no
H71B	H8	2.5595	.	2_675	no
H72	H69	2.4284	.	2_665	no
H72B	H69	2.5156	.	2_665	no
H73	H69	2.5268	.	2_665	no
H73B	C60	3.0622	.	1_645	no
H74B	C23	3.0081	.	1_645	no
H74B	H23'	2.5458	.	2_665	no
H75	H47	2.5669	.	.	no
H75B	H47"	2.2251	.	.	no
H75B	C47	2.6319	.	.	no

H75B	H47	2.2125	.	.	no
H76	H47"	2.4995	.	2_665	no

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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

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#
#D   H   A   D - H   H...A   D...A   D - H...A   symm(A)
#
C7      H7      O2      1.0000   2.5708   3.173(3)   118.56   .   yes
C19     H19     O4      1.0001   2.5067   3.133(2)   120.32   .   yes
C22     H22     O3      1.0001   2.5750   3.161(3)   117.27   .   yes
C46     H46     O7      1.0006   2.5209   3.299(3)   134.39   .   yes

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# End of Crystallographic Information File

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