

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cueu

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cueu

Bond precision: C-C = 0.0112 Å Wavelength=0.71073

Cell: a=13.952(2) b=13.952(2) c=22.836(4)
 alpha=90 beta=90 gamma=120
Temperature: 150 K

	Calculated	Reported
Volume	3849.7(15)	3849.6(13)
Space group	P 32 2 1	P 32 2 1
Hall group	P 32 2 "	P 32 2 "
Moiety formula	C30 H34 Cl2 Cu2 Eu N11 O13, 2(C3 H6 N O), H2 O	C30 H34 Cl2 Cu2 Eu N11 O13, 2(C3 H6 N O), H2 O
Sum formula	C36 H48 Cl2 Cu2 Eu N13 O16	C36 H48 Cl2 Cu2 Eu N13 O16
Mr	1268.84	1268.81
Dx,g cm-3	1.642	1.642
Z	3	3
Mu (mm-1)	2.208	2.208
F000	1914.0	1914.0
F000'	1917.05	
h,k,lmax	18,18,29	17,18,29
Nref	5964[3339]	5900
Tmin,Tmax	0.498,0.629	0.607,0.746
Tmin'	0.488	

Correction method= # Reported T Limits: Tmin=0.607 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.99 Theta(max)= 27.590

R(reflections)= 0.0449(5324) wR2(reflections)= 0.1179(5900)

S = 1.022 Npar= 313

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.6 Ratio

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.320

From the CIF: _refine_ls_abs_structure_Flack_su 0.020

PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio 3.1 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 N Ueq(max)/Ueq(min) Range 5.6 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 6.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N2 --C2 . 5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O3 --C1 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --C3 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Eu1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C16 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N7 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.5 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O8A 0.135 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01125 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C30 H34 Cl2 Cu2 Eu N11 O13
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H1 -0.36 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.320 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.51 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 5 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 4 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O1 --N1_f . 5.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H10B	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	3%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	20%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C18	Check
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O8A	61.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O8B	67.8	Degree
PLAT721_ALERT_1_G	Bond Calc	0.97000, Rep 0.96000 Dev...	0.01	Ang.
	C17 -H17B	1.555 1.555	# 79	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)		1.20	Ratio
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Eu1	--Cu1 ..	9.05	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Eu1	--Cu1 ..	4.20	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Cu1	--Cu1 ..	10.77	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Cu1	--Cu1 ..	7.05	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	97	Check
	N1 -O1 -N1	1.555 1.555 6.556	21.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	100	Check
	N1 -O2 -N1	1.555 1.555 6.556	30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	121	Check
	N1 -N1 -O1	6.556 1.555 6.556	23.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	209	Check
	H10B -O10 -H10B	1.555 1.555 1.555	0.00	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	2	Note
	C3 H6 N O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	3	Note
	H2 O			
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1	(II) .	2.10	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		36	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	26	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 42 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 29 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL002_ALERT_1_A The contact author's address is missing,
 _publ_contact_author_address.
 PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
 PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
 PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
 PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
 PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
```

```

_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_ABSTY02_cueu
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_STRVA01_cueu
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT213_cueu
;
PROBLEM: Atom C1                has ADP max/min Ratio .....      3.1 prolat
RESPONSE: ...
;
_vrf_PLAT220_cueu
;
PROBLEM: Non-Solvent  Resd 1  N    Ueq(max)/Ueq(min) Range      5.6 Ratio
RESPONSE: ...
;
_vrf_PLAT222_cueu
;
PROBLEM: Non-Solv.  Resd 1  H    Uiso(max)/Uiso(min) Range      6.5 Ratio
RESPONSE: ...
;
_vrf_PLAT230_cueu
;
PROBLEM: Hirshfeld Test Diff for    N2      --C2      .      5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT234_cueu
;
PROBLEM: Large Hirshfeld Difference O3      --C1      .      0.20 Ang.
RESPONSE: ...
;
_vrf_PLAT241_cueu
;
PROBLEM: High    'MainMol' Ueq as Compared to Neighbors of      01 Check
RESPONSE: ...
;
_vrf_PLAT242_cueu
;
PROBLEM: Low     'MainMol' Ueq as Compared to Neighbors of      Eu1 Check
RESPONSE: ...
;
_vrf_PLAT243_cueu
;
PROBLEM: High    'Solvent' Ueq as Compared to Neighbors of      C16 Check
RESPONSE: ...
;
_vrf_PLAT244_cueu
;

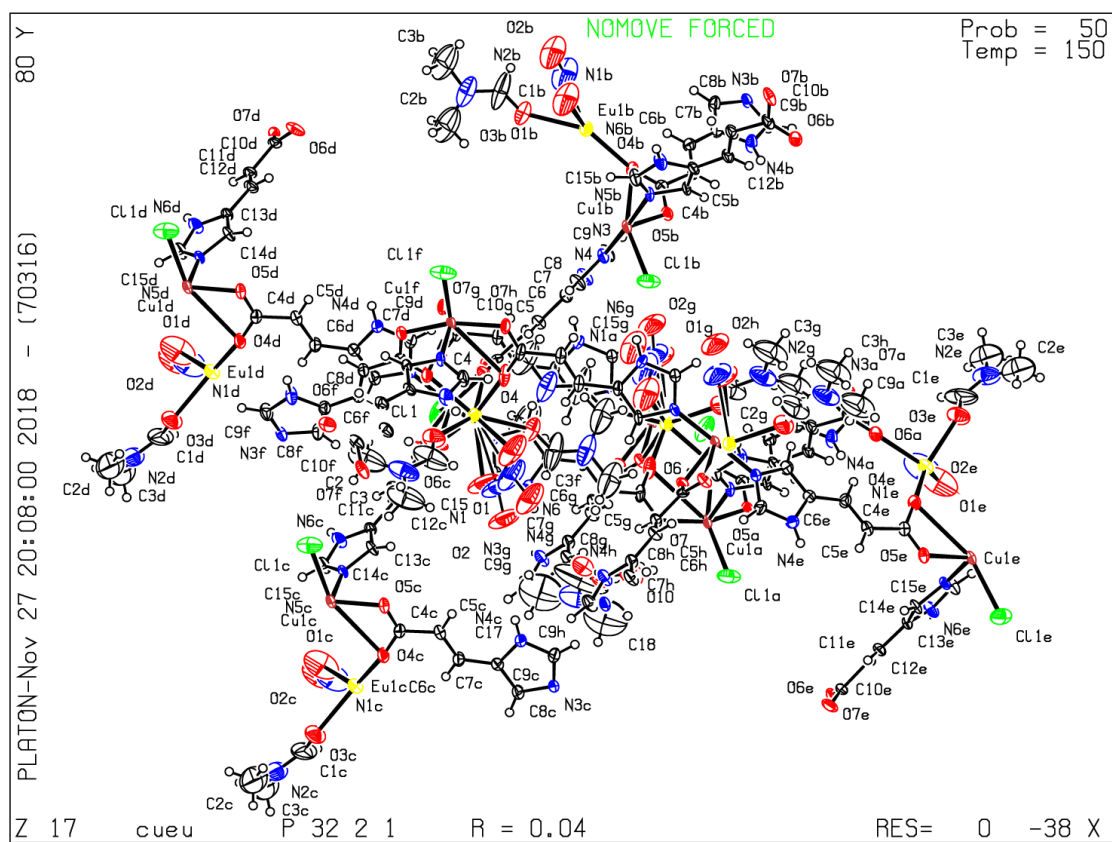
```

```

PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of      N7 Check
RESPONSE: ...
;
_vrf_PLAT250_cueu
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      3.5 Note
RESPONSE: ...
;
_vrf_PLAT260_cueu
;
PROBLEM: Large Average Ueq of Residue Including      O8A      0.135 Check
RESPONSE: ...
;
_vrf_PLAT342_cueu
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.01125 Ang.
RESPONSE: ...
;
_vrf_PLAT790_cueu
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #      1 Note
RESPONSE: ...
;
_vrf_PLAT934_cueu
;
PROBLEM: Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....      1 Check
RESPONSE: ...
;
_vrf_PLAT977_cueu
;
PROBLEM: Check Negative Difference Density on H1      -0.36 eA-3
RESPONSE: ...
;
_vrf_PLAT978_cueu
;
PROBLEM: Number C-C Bonds with Positive Residual Density.      0 Info
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.



```

data_cueu

_audit_update_record
;
2018-11-27 # Formatted by publCIF

;
_audit_creation_date          2018-11-27
_audit_creation_method
;
Olex2 1.2
(compiled 2017.03.28 svn.r3405 for OlexSys, GUI svn.r5335)
;
_shelx_SHELXL_version_number  '2014/7'
loop_
  _publ_body_element
  _publ_body_title
  _publ_body_contents
section
;
Introduction
;
;

;
section
;
Experimental
;
;

;
subsection
;
Synthesis and crystallization
;
;

;
subsection
;
Refinement
;
;
Crystal data, data collection and structure refinement details are
summarized
in Table 1.
;
section
;
Results and discussion
;
;

```


;

_publ_contact_author_address ?
_publ_contact_author_email ?
_publ_contact_author_id_orcid ?
_publ_contact_author_name ''
_publ_contact_author_phone ?
_publ_section_references
;

Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacobazzi, C., Polidori, G., Siliqi, D. & Spagna, R. (2007). *J. Appl. Cryst.* **40**, 609--613.

Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacobazzi, C., Polidori, G., Siliqi, D. & Spagna, R. (2007). *J. Appl. Cryst.* **40**, 609--613.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339--341.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339--341.

Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3--8.

Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3--8.

;

_chemical_name_common ?
_chemical_name_systematic ?
_chemical_formula_moiety 'C30 H34 Cl2 Cu2 Eu N11 O13, 2(C3 H6 N O), H2 O'
_chemical_formula_sum 'C36 H48 Cl2 Cu2 Eu N13 O16'
_chemical_formula_weight 1268.81
_chemical_absolute_configuration ?
_chemical_melting_point ?
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
'C' 'C' 0.0033 0.0016 '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'
'Cl' 'Cl' 0.1484 0.1585 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Cu' 'Cu' 0.3201 1.2651 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Eu' 'Eu' -0.1578 3.6682
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N' 'N' 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O' 'O' 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_shelx_space_group_comment

;

The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names. They are only intended as comments.

;

_space_group_crystal_system trigonal
 _space_group_IT_number 154
 _space_group_name_H-M_alt 'P 32 2 1'
 _space_group_name_Hall 'P 32 2''
 loop_
 _space_group_symop_operation_xyz
 'x, y, z'
 '-y, x-y, z+2/3'
 '-x+y, -x, z+1/3'
 'y, x, -z'
 'x-y, -y, -z+1/3'
 '-x, -x+y, -z+2/3'

_cell_length_a 13.952(2)
 _cell_length_b 13.952(2)
 _cell_length_c 22.836(4)
 _cell_angle_alpha 90
 _cell_angle_beta 90
 _cell_angle_gamma 120
 _cell_volume 3849.6(13)
 _cell_formula_units_Z 3
 _cell_measurement_reflns_used 9774
 _cell_measurement_temperature 150(2)
 _cell_measurement_theta_max 27.47
 _cell_measurement_theta_min 2.45
 _shelx_estimated_absorpt_T_max ?
 _shelx_estimated_absorpt_T_min ?
 _exptl_absorpt_coefficient_mu 2.208
 _exptl_absorpt_correction_T_max ?
 _exptl_absorpt_correction_T_min ?
 _exptl_absorpt_correction_type multi-scan
 _exptl_absorpt_process_details ?
 _exptl_absorpt_special_details ?
 _exptl_crystal_colour blue
 _exptl_crystal_colour_primary blue
 _exptl_crystal_density_diffn 1.642
 _exptl_crystal_density_meas ?
 _exptl_crystal_density_method ?

```

_exptl_crystal_description      prism
_exptl_crystal_F_000           1914
_exptl_crystal_size_max        0.32
_exptl_crystal_size_mid        0.28
_exptl_crystal_size_min        0.21
_exptl_transmission_factor_max  0.7456
_exptl_transmission_factor_min  0.6069
_diffn_reflns_av_R_equivalents 0.0445
_diffn_reflns_av_unetI/netI    0.0636
_diffn_reflns_Laue_measured_fraction_full 0.999
_diffn_reflns_Laue_measured_fraction_max 0.991
_diffn_reflns_limit_h_max      17
_diffn_reflns_limit_h_min      -17
_diffn_reflns_limit_k_max      18
_diffn_reflns_limit_k_min      -18
_diffn_reflns_limit_l_max      29
_diffn_reflns_limit_l_min      0
_diffn_reflns_number           15707
_diffn_reflns_point_group_measured_fraction_full 0.999
_diffn_reflns_point_group_measured_fraction_max 0.991
_diffn_reflns_theta_full       25.242
_diffn_reflns_theta_max        27.590
_diffn_reflns_theta_min        2.454
_diffn_ambient_temperature     150(2)
_diffn_detector_area_resol_mean ?
_diffn_measured_fraction_theta_full 0.999
_diffn_measured_fraction_theta_max 0.991
_diffn_measurement_device_type  'D8 VENTURE Bruker AXS'
_diffn_measurement_method      'rotation images'
_diffn_radiation_type          MoK\alpha
_diffn_radiation_wavelength    0.71073
_diffn_source                   'Incoatec microfocus sealed tube'
_reflns_Friedel_coverage       0.786
_reflns_Friedel_fraction_full  1.000
_reflns_Friedel_fraction_max   0.991
_reflns_number_gt              5324
_reflns_number_total           5900
_reflns_special_details

;
Reflections were merged by SHELXL according to the crystal
class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique
Friedel pairs measured divided by the number that would be
possible theoretically, ignoring centric projections and
systematic absences.

;
_reflns_threshold_expression    'I > 2\sigma(I)'
_computing_cell_refinement      'APEX3 (Bruker, 2015); SAINT (Bruker,
2014)'
_computing_data_collection      'SAINT (Bruker, 2014)'
_computing_data_reduction       'SAINT (Bruker, 2014)'
_computing_molecular_graphics   'Olex2 (Dolomanov et al., 2009)'
_computing_publication_material 'Olex2 (Dolomanov et al., 2009)'

```

```

_computing_structure_refinement 'ShelXL (Sheldrick, 2015)'
_computing_structure_solution 'SIR2004 (Burla et al., 2007)'
_refine_diff_density_max 1.094
_refine_diff_density_min -1.599
_refine_diff_density_rms 0.124
_refine_ls_abs_structure_details
;
  Refined as an inversion twin.
;
_refine_ls_abs_structure_Flack 0.32(2)
_refine_ls_extinction_coef .
_refine_ls_extinction_method none
_refine_ls_goodness_of_fit_ref 1.022
_refine_ls_hydrogen_treatment constr
_refine_ls_matrix_type full
_refine_ls_number_parameters 313
_refine_ls_number_reflns 5900
_refine_ls_number_restraints 36
_refine_ls_R_factor_all 0.0550
_refine_ls_R_factor_gt 0.0449
_refine_ls_restrained_S_all 1.022
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000
_refine_ls_structure_factor_coef Fsqd
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0557P)^2^+6.5149P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_weighting_scheme calc
_refine_ls_wR_factor_gt 0.1116
_refine_ls_wR_factor_ref 0.1179
_refine_special_details
;
  Refined as a 2-component inversion twin.
;
_olex2_refinement_description
;
1. Twinned data refinement
  Scales: 0.68(2)
  0.32(2)
2. Fixed Uiso
  At 1.2 times of:
    All C(H) groups, All N(H) groups
  At 1.5 times of:
    All C(H,H,H) groups, All O(H,H) groups
3. Restrained distances
  O10-H10A
  0.85 with sigma of 0.001
  O10-H10B
  0.85 with sigma of 0.02
4. Restrained planarity
  C11, H11, C12, H12
  with sigma of 0.1
5. Rigid bond restraints
  O1, O2, N1
  with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01

```

6. Uiso/Uanis restraints and constraints

O10: within 1.7Å with sigma of 0.04 and sigma for terminal atoms of 0.08
Uanis(C16) \\sim Ueq, Uanis(N7) \\sim Ueq: with sigma of 0.1 and sigma
for
terminal atoms of 0.2
Uanis(O1) \\sim Ueq, Uanis(N1) \\sim Ueq: with sigma of 0.1 and sigma for
terminal atoms of 0.2
Uanis(O10) \\sim Ueq: with sigma of 0.05 and sigma for terminal atoms of
0.1
Uanis(O10) \\sim Ueq, : with sigma of 0.05 and sigma for terminal atoms
of 0.01
Uanis(C18) = Uanis(C17)
Uanis(C2) = Uanis(C3)
Uanis(O1) = Uanis(O2)
Uanis(O8A) = Uanis(O8B)
Uanis(N1) = Uanis(O1)

7. Others

Fixed Sof: O2(0.5) N1(0.5) O8A(0.5) O8B(0.5) H10A(0.5) H10B(0.5)

8.a Free rotating group:

O10(H10A,H10B)

8.b Aromatic/amide H refined with riding coordinates:

N4(H4), N6(H6), C1(H1), C5(H5), C6(H6A), C8(H8), C9(H9), C11(H11),
C12(H12),
C14(H14), C15(H15)

8.c Idealised Me refined as rotating group:

C2(H2A,H2B,H2C), C3(H3A,H3B,H3C), C17(H17A,H17B,H17C),
C18(H18A,H18B,H18C)

;

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_atom_sites_solution_primary	direct
_atom_sites_solution_secondary	?

loop_

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_atom_site_fract_y	
_atom_site_fract_z	
_atom_site_U_iso_or_equiv	
_atom_site_adp_type	
_atom_site_occupancy	
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_atom_site_refinement_flags_occupancy	
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_atom_site_disorder_group	

Eu1	Eu	0.0000	0.64929(4)	0.8333	0.02949(16)	Uani	1	2	d	S	T	P	.	.	.
Cu1	Cu	-0.29160(8)	0.66729(7)	0.83765(3)	0.0193(2)	Uani	1	1	d
C11	C1	-0.4849(2)	0.6410(2)	0.84457(12)	0.0566(7)	Uani	1	1	d
O1	O	-0.0782(13)	0.4464(8)	0.8599(6)	0.115(5)	Uani	1	1	d	.	U
O2	O	-0.037(2)	0.3340(16)	0.8564(10)	0.115(5)	Uani	0.5	1	d	.	U
O3	O	0.1022(7)	0.6427(7)	0.9176(3)	0.056(2)	Uani	1	1	d
O4	O	-0.0744(4)	0.7440(5)	0.7844(2)	0.0286(12)	Uani	1	1	d

O5 O -0.2263(4) 0.7490(4) 0.76225(19) 0.0240(10) Uani 1 1 d
 O6 O -0.5931(5) 0.2551(6) 0.5598(2) 0.0376(15) Uani 1 1 d
 O7 O -0.5844(4) 0.1043(5) 0.5817(2) 0.0297(12) Uani 1 1 d
 N2 N 0.1759(9) 0.5936(11) 0.9909(5) 0.080(4) Uani 1 1 d
 N1 N -0.026(4) 0.427(2) 0.8460(18) 0.115(5) Uani 0.5 1 d . U . . .
 N3 N 0.1916(5) 0.9701(5) 0.5482(2) 0.0229(12) Uani 1 1 d
 N4 N 0.0202(6) 0.9122(6) 0.5755(2) 0.0317(15) Uani 1 1 d
 H4 H -0.0471 0.8985 0.5742 0.038 Uiso 1 1 calc R
 N5 N -0.3499(5) 0.5288(5) 0.7927(2) 0.0203(12) Uani 1 1 d
 N6 N -0.4270(6) 0.3528(5) 0.7687(2) 0.0298(14) Uani 1 1 d
 H6 H -0.4508 0.2830 0.7718 0.036 Uiso 1 1 calc R
 C1 C 0.1458(12) 0.5965(16) 0.9386(7) 0.110(7) Uani 1 1 d
 H1 H 0.1606 0.5549 0.9121 0.132 Uiso 1 1 calc R
 C2 C 0.1661(16) 0.6615(18) 1.0372(9) 0.126(6) Uani 1 1 d
 H2A H 0.2379 0.7106 1.0533 0.189 Uiso 1 1 calc GR
 H2B H 0.1183 0.6142 1.0676 0.189 Uiso 1 1 calc GR
 H2C H 0.1356 0.7040 1.0210 0.189 Uiso 1 1 calc GR
 C3 C 0.2176(16) 0.5247(17) 1.0090(9) 0.126(6) Uani 1 1 d
 H3A H 0.2040 0.4712 0.9790 0.189 Uiso 1 1 calc GR
 H3B H 0.1813 0.4872 1.0445 0.189 Uiso 1 1 calc GR
 H3C H 0.2958 0.5688 1.0158 0.189 Uiso 1 1 calc GR
 C4 C -0.1324(7) 0.7640(6) 0.7500(3) 0.0189(12) Uani 1 1 d
 C5 C -0.0868(6) 0.8112(6) 0.6912(3) 0.0247(14) Uani 1 1 d
 H5 H -0.1309 0.8232 0.6651 0.030 Uiso 1 1 calc R
 C6 C 0.0141(6) 0.8367(6) 0.6750(3) 0.0255(15) Uani 1 1 d
 H6A H 0.0545 0.8205 0.7015 0.031 Uiso 1 1 calc R
 C7 C 0.0688(6) 0.8871(7) 0.6204(3) 0.0234(14) Uani 1 1 d
 C8 C 0.1742(7) 0.9227(7) 0.6029(3) 0.0312(18) Uani 1 1 d
 H8 H 0.2270 0.9161 0.6247 0.037 Uiso 1 1 calc R
 C9 C 0.0982(7) 0.9626(8) 0.5334(3) 0.0339(19) Uani 1 1 d
 H9 H 0.0862 0.9887 0.4983 0.041 Uiso 1 1 calc R
 C10 C -0.5677(7) 0.1992(8) 0.5933(3) 0.0267(15) Uani 1 1 d
 C11 C -0.5122(6) 0.2504(7) 0.6504(3) 0.0271(17) Uani 1 1 d
 H11 H -0.4987 0.2080 0.6769 0.032 Uiso 1 1 calc R
 C12 C -0.4820(6) 0.3534(7) 0.6641(3) 0.0272(16) Uani 1 1 d
 H12 H -0.4933 0.3953 0.6361 0.033 Uiso 1 1 calc R
 C13 C -0.4325(6) 0.4069(6) 0.7193(3) 0.0228(15) Uani 1 1 d
 C14 C -0.3848(7) 0.5149(6) 0.7348(3) 0.0240(15) Uani 1 1 d
 H14 H -0.3765 0.5716 0.7102 0.029 Uiso 1 1 calc R
 C15 C -0.3780(7) 0.4283(6) 0.8109(3) 0.0302(17) Uani 1 1 d
 H15 H -0.3653 0.4120 0.8487 0.036 Uiso 1 1 calc R
 O8A O -0.0659(13) 0.1204(15) 0.7687(7) 0.048(3) Uani 0.5 1 d
 O8B O -0.1048(15) 0.0650(15) 0.7457(7) 0.048(3) Uani 0.5 1 d
 N7 N -0.2527(10) 0.0218(15) 0.7807(10) 0.113(6) Uani 1 1 d . U . . .
 C16 C -0.1510(16) 0.078(3) 0.7732(14) 0.197(16) Uani 1 1 d . U . . .
 C17 C -0.279(3) 0.069(3) 0.8317(14) 0.198(9) Uani 1 1 d
 H17A H -0.3037 0.0170 0.8635 0.298 Uiso 1 1 calc GR
 H17B H -0.3373 0.0841 0.8215 0.298 Uiso 1 1 calc GR
 H17C H -0.2148 0.1364 0.8434 0.298 Uiso 1 1 calc GR
 C18 C -0.330(3) -0.072(3) 0.7482(13) 0.198(9) Uani 1 1 d
 H18A H -0.2928 -0.0868 0.7173 0.298 Uiso 1 1 calc GR
 H18B H -0.3854 -0.0581 0.7318 0.298 Uiso 1 1 calc GR
 H18C H -0.3654 -0.1353 0.7737 0.298 Uiso 1 1 calc GR
 O10 O -0.5011(9) 0.0000 0.6667 0.074(3) Uani 1 2 d DS TU P . .

H10A H -0.5480 0.0033 0.6442 0.111 Uiso 0.5 1 d DG U . . .
H10B H -0.5184 -0.0161 0.6305 0.111 Uiso 0.5 1 d DG U . . .

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Cu1 0.0284(4) 0.0181(4) 0.0106(3) -0.0002(3) -0.0016(3) 0.0110(3)
Cl1 0.0386(13) 0.0638(15) 0.0770(16) -0.0384(13) -0.0124(11) 0.0327(12)
O1 0.167(12) 0.039(4) 0.141(9) -0.011(4) -0.067(8) 0.053(5)
O2 0.167(12) 0.039(4) 0.141(9) -0.011(4) -0.067(8) 0.053(5)
O3 0.055(5) 0.057(5) 0.056(4) 0.011(4) -0.017(3) 0.028(4)
O4 0.031(3) 0.037(3) 0.020(2) 0.009(2) 0.0026(19) 0.019(3)
O5 0.033(3) 0.025(3) 0.015(2) 0.0047(18) 0.0042(18) 0.016(2)
O6 0.036(3) 0.059(5) 0.028(3) -0.022(3) -0.018(2) 0.031(3)
O7 0.026(3) 0.032(3) 0.014(2) -0.0067(19) -0.0008(19) 0.002(2)
N2 0.048(6) 0.085(8) 0.088(7) 0.044(6) -0.011(5) 0.019(6)
N1 0.167(12) 0.039(4) 0.141(9) -0.011(4) -0.067(8) 0.053(5)
N3 0.021(3) 0.031(3) 0.014(2) 0.000(2) 0.001(2) 0.010(3)
N4 0.021(3) 0.047(4) 0.020(3) 0.010(3) 0.001(2) 0.012(3)
N5 0.025(3) 0.024(3) 0.011(2) 0.002(2) -0.003(2) 0.011(3)
N6 0.042(4) 0.017(3) 0.022(3) -0.008(2) -0.009(3) 0.008(3)
C1 0.053(8) 0.128(15) 0.108(12) 0.064(11) -0.033(8) 0.014(9)
C2 0.092(9) 0.134(13) 0.140(12) 0.072(10) 0.001(8) 0.047(9)
C3 0.092(9) 0.134(13) 0.140(12) 0.072(10) 0.001(8) 0.047(9)
C4 0.026(4) 0.011(3) 0.020(3) 0.002(3) 0.003(3) 0.009(2)
C5 0.032(4) 0.027(4) 0.016(3) 0.001(3) -0.001(3) 0.016(3)
C6 0.027(4) 0.032(4) 0.021(3) 0.006(3) 0.004(3) 0.017(3)
C7 0.023(4) 0.028(4) 0.020(3) 0.001(3) -0.001(3) 0.013(3)
C8 0.028(4) 0.044(5) 0.021(3) 0.010(3) 0.001(3) 0.018(4)
C9 0.025(4) 0.050(5) 0.024(3) 0.010(3) 0.007(3) 0.017(4)
C10 0.019(4) 0.035(4) 0.019(3) -0.013(3) -0.005(3) 0.008(3)
C11 0.021(4) 0.037(5) 0.019(3) -0.009(3) -0.004(3) 0.012(3)
C12 0.027(4) 0.036(4) 0.019(3) -0.011(3) -0.007(3) 0.016(3)
C13 0.024(4) 0.029(4) 0.014(3) -0.007(3) -0.002(3) 0.013(3)
C14 0.036(4) 0.029(4) 0.011(3) -0.006(2) -0.008(3) 0.020(3)
C15 0.046(5) 0.023(4) 0.017(3) -0.002(3) -0.006(3) 0.014(3)
O8A 0.042(7) 0.062(10) 0.053(8) 0.014(5) 0.011(5) 0.036(7)
O8B 0.042(7) 0.062(10) 0.053(8) 0.014(5) 0.011(5) 0.036(7)
N7 0.047(7) 0.099(11) 0.177(16) 0.053(11) 0.000(8) 0.025(7)
C16 0.073(12) 0.26(3) 0.27(3) 0.21(3) 0.066(16) 0.093(17)
C17 0.17(2) 0.23(3) 0.23(3) 0.05(2) -0.024(19) 0.12(2)
C18 0.17(2) 0.23(3) 0.23(3) 0.05(2) -0.024(19) 0.12(2)
O10 0.064(5) 0.111(9) 0.064(7) 0.016(7) 0.008(3) 0.055(4)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop_

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Eu1 Cu1 9.0456(15) 5_666 ?

Eu1 Cu1 4.2007(12) . ?

Eu1 O1 2.546(10) . ?

Eu1 O1 2.546(10) 6_556 ?

Eu1 O3 2.424(7) 6_556 ?

Eu1 O3 2.424(7) . ?

Eu1 O4 2.333(5) . ?

Eu1 O4 2.333(5) 6_556 ?

Eu1 O6 2.303(6) 3_455 ?

Eu1 O6 2.303(6) 5_666 ?

Eu1 N1 2.95(2) 6_556 ?

Eu1 N1 2.95(2) . ?

Cu1 Cu1 10.7679(16) 3_455 ?

Cu1 Cu1 7.049(2) 6_556 ?

Cu1 C11 2.539(3) . ?

Cu1 O5 2.014(5) . ?

Cu1 O7 2.054(5) 3_455 ?

Cu1 N3 1.977(6) 3_465 ?

Cu1 N5 1.969(6) . ?

O1 N1 1.67(4) 6_556 ?

O1 N1 0.95(4) . ?

O2 O2 1.38(6) 6_556 ?

O2 N1 1.65(4) 6_556 ?

O2 N1 1.25(3) . ?

O3 C1 1.188(18) . ?

O4 C4 1.256(8) . ?

O5 C4 1.251(9) . ?

O6 Eu1 2.303(6) 2_564 ?

O6 C10 1.264(10) . ?

O7 Cu1 2.054(5) 2_564 ?

O7 C10 1.252(10) . ?

N2 C1 1.273(17) . ?

N2 C2 1.47(2) . ?

N2 C3 1.41(2) . ?

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N1 O2 1.65(4) 6_556 ?

N1 N1 0.85(8) 6_556 ?

N3 Cu1 1.977(6) 2_674 ?

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N3 C9 1.300(11) . ?

N4 H4 0.8600 . ?
N4 C7 1.368(9) . ?
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N6 C15 1.336(9) . ?
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C2 H2B 0.9600 . ?
C2 H2C 0.9600 . ?
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C3 H3B 0.9600 . ?
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C5 C6 1.321(11) . ?
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C7 C8 1.356(11) . ?
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C15 H15 0.9300 . ?
O8A O8B 0.865(19) . ?
O8A C16 1.03(2) . ?
O8B C16 0.98(3) . ?
N7 C16 1.24(2) . ?
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N7 C18 1.42(3) . ?
C17 H17A 0.9600 . ?
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C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
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O6 Eu1 O4 85.9(2) 3_455 6_556 ?
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 Eu1 Cu1 Cu1 32.956(13) . 6_556 ?
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 C11 Cu1 Eu1 169.61(8) . . ?
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 O7 Cu1 C11 91.82(19) 3_455 . ?
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 N3 Cu1 C11 94.2(2) 3_465 . ?
 N3 Cu1 O5 90.6(2) 3_465 . ?
 N3 Cu1 O7 89.1(2) 3_465 3_455 ?
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 N5 Cu1 Cu1 88.07(16) . 3_455 ?
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17 -5 8 65.92 34.21

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_iucr_refine_instructions_details
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cueu.res created by SHELXL-2014/7

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TITL shelxs86_a.res in P3(2)21
CELL 0.71073 13.952 13.9516 22.836 90 90 120
ZERR 3 0.002 0.002 0.004 0 0 0
LATT -1
SYMM -Y,+X-Y,0.667+Z
SYMM +Y-X,-X,0.333+Z
SYMM +Y,+X,-Z
SYMM -Y+X,-Y,0.333-Z
SYMM -X,-X+Y,0.667-Z
SFAC C H Cl Cu Eu N O
UNIT 108 144 6 6 3 39 48
EQIV $1 1-Y+X,1-Y,1.333-Z
EQIV $2 -X,-X+Y,1.667-Z
EQIV $3 -1+Y-X,-X,0.333+Z
EQIV $4 -Y+X,1-Y,1.333-Z
DFIX 0.85 0.001 O10 H10a
DFIX 0.85 O10 H10b
FLAT C11 H11 C12 H12
DELU O1 O2 N1
SIMU 0.04 0.08 1.7 O10
ISOR C16 N7
ISOR O1 N1
ISOR 0.05 0.1 O10
ISOR 0.05 0.01 O10 H10b H10a

```

EADP C18 C17
EADP C2 C3
EADP O1 O2
EADP O8A O8B
EADP N1 O1

L.S. 100
PLAN 20
HTAB N4 O8A_\$4
HTAB N4 O8B_\$4
BIND Cu1 Cu1_\$2
BIND Cu1 Cu1_\$3
BIND Eu1 Cu1
BIND Eu1 Cu1_\$1
BIND O10 H10b
BOND \$H
list 4
fmap -2
acta
TWIN -1 0 0 0 -1 0 0 0 -1 2
REM <olex2.extras>
REM <HklSrc "%.\cueu.hkl">
REM </olex2.extras>

WGHT	0.055700	6.514900				
BASF	0.31769					
FVAR	0.16766					
EU1	5	0.000000	0.649295	0.833333	10.50000	0.03478
0.02874 =						
		0.02697	-0.00293	-0.00587	0.01739	
CU1	4	-0.291600	0.667288	0.837648	11.00000	0.02837
0.01814 =						
		0.01057	-0.00024	-0.00163	0.01097	
CL1	3	-0.484914	0.641025	0.844569	11.00000	0.03856
0.06381 =						
		0.07704	-0.03844	-0.01240	0.03273	
O1	7	-0.078221	0.446390	0.859915	11.00000	0.16717
0.03909 =						
		0.14131	-0.01071	-0.06654	0.05264	
O2	7	-0.036619	0.334000	0.856403	10.50000	0.16717
0.03909 =						
		0.14131	-0.01071	-0.06654	0.05264	
O3	7	0.102159	0.642716	0.917635	11.00000	0.05498
0.05746 =						
		0.05568	0.01084	-0.01745	0.02753	
O4	7	-0.074367	0.743995	0.784364	11.00000	0.03127
0.03651 =						
		0.02026	0.00897	0.00259	0.01873	
O5	7	-0.226347	0.748993	0.762246	11.00000	0.03293
0.02547 =						
		0.01519	0.00471	0.00420	0.01578	
O6	7	-0.593052	0.255097	0.559760	11.00000	0.03581
0.05861 =						
		0.02828	-0.02160	-0.01778	0.03094	

O7	7	-0.584421	0.104301	0.581709	11.00000	0.02571
0.03236 =						
		0.01391	-0.00668	-0.00079	0.00176	
N2	6	0.175903	0.593624	0.990924	11.00000	0.04761
0.08497 =						
		0.08845	0.04381	-0.01149	0.01940	
N1	6	-0.025643	0.427138	0.846012	10.50000	0.16717
0.03909 =						
		0.14131	-0.01071	-0.06654	0.05264	
N3	6	0.191645	0.970131	0.548192	11.00000	0.02054
0.03059 =						
		0.01365	0.00032	0.00078	0.00993	
N4	6	0.020224	0.912196	0.575494	11.00000	0.02082
0.04740 =						
		0.02021	0.00965	0.00089	0.01199	
AFIX	43					
H4	2	-0.047062	0.898539	0.574198	11.00000	-1.20000
AFIX	0					
N5	6	-0.349852	0.528846	0.792694	11.00000	0.02457
0.02433 =						
		0.01085	0.00216	-0.00283	0.01135	
N6	6	-0.426990	0.352810	0.768717	11.00000	0.04169
0.01681 =						
		0.02168	-0.00765	-0.00907	0.00762	
AFIX	43					
H6	2	-0.450817	0.283025	0.771763	11.00000	-1.20000
AFIX	0					
C1	1	0.145805	0.596451	0.938621	11.00000	0.05326
0.12757 =						
		0.10820	0.06394	-0.03312	0.01424	
AFIX	43					
H1	2	0.160643	0.554887	0.912139	11.00000	-1.20000
AFIX	0					
C2	1	0.166071	0.661481	1.037237	11.00000	0.09160
0.13370 =						
		0.13974	0.07220	0.00120	0.04704	
AFIX	137					
H2A	2	0.237921	0.710561	1.053282	11.00000	-1.50000
H2B	2	0.118269	0.614166	1.067617	11.00000	-1.50000
H2C	2	0.135606	0.704004	1.021041	11.00000	-1.50000
AFIX	0					
C3	1	0.217600	0.524701	1.008976	11.00000	0.09160
0.13370 =						
		0.13974	0.07220	0.00120	0.04704	
AFIX	137					
H3A	2	0.204024	0.471171	0.978973	11.00000	-1.50000
H3B	2	0.181344	0.487210	1.044462	11.00000	-1.50000
H3C	2	0.295791	0.568848	1.015769	11.00000	-1.50000
AFIX	0					
C4	1	-0.132418	0.764004	0.749957	11.00000	0.02566
0.01128 =						
		0.01988	0.00155	0.00350	0.00943	
C5	1	-0.086810	0.811224	0.691210	11.00000	0.03218
0.02712 =						

		0.01634	0.00097	-0.00128	0.01605	
AFIX	43					
H5	2	-0.130899	0.823163	0.665071	11.00000	-1.20000
AFIX	0					
C6	1	0.014111	0.836729	0.674954	11.00000	0.02732
0.03151	=					
		0.02078	0.00640	0.00363	0.01695	
AFIX	43					
H6A	2	0.054470	0.820481	0.701548	11.00000	-1.20000
AFIX	0					
C7	1	0.068774	0.887097	0.620410	11.00000	0.02287
0.02797	=					
		0.02005	0.00147	-0.00069	0.01316	
C8	1	0.174220	0.922695	0.602923	11.00000	0.02819
0.04381	=					
		0.02148	0.00981	0.00134	0.01796	
AFIX	43					
H8	2	0.226971	0.916062	0.624667	11.00000	-1.20000
AFIX	0					
C9	1	0.098153	0.962626	0.533442	11.00000	0.02520
0.05030	=					
		0.02378	0.00955	0.00683	0.01704	
AFIX	43					
H9	2	0.086221	0.988707	0.498295	11.00000	-1.20000
AFIX	0					
C10	1	-0.567700	0.199174	0.593309	11.00000	0.01917
0.03469	=					
		0.01930	-0.01342	-0.00543	0.00830	
C11	1	-0.512192	0.250398	0.650362	11.00000	0.02134
0.03738	=					
		0.01922	-0.00915	-0.00394	0.01222	
AFIX	43					
H11	2	-0.498679	0.207977	0.676909	11.00000	-1.20000
AFIX	0					
C12	1	-0.481982	0.353422	0.664081	11.00000	0.02656
0.03634	=					
		0.01926	-0.01075	-0.00650	0.01603	
AFIX	43					
H12	2	-0.493272	0.395271	0.636137	11.00000	-1.20000
AFIX	0					
C13	1	-0.432463	0.406941	0.719329	11.00000	0.02393
0.02922	=					
		0.01426	-0.00718	-0.00224	0.01254	
C14	1	-0.384760	0.514881	0.734803	11.00000	0.03644
0.02944	=					
		0.01096	-0.00570	-0.00791	0.02012	
AFIX	43					
H14	2	-0.376546	0.571587	0.710167	11.00000	-1.20000
AFIX	0					
C15	1	-0.378030	0.428285	0.810946	11.00000	0.04588
0.02325	=					
		0.01685	-0.00188	-0.00615	0.01372	
AFIX	43					
H15	2	-0.365324	0.411972	0.848650	11.00000	-1.20000

```

AFIX 0

O8A 7 -0.065888 0.120378 0.768735 10.50000 0.04191
0.06219 =
      0.05331 0.01431 0.01079 0.03575
O8B 7 -0.104839 0.065013 0.745704 10.50000 0.04191
0.06219 =
      0.05331 0.01431 0.01079 0.03575
N7 6 -0.252667 0.021813 0.780671 11.00000 0.04719
0.09868 =
      0.17696 0.05297 0.00044 0.02511
C16 1 -0.151041 0.077627 0.773161 11.00000 0.07301
0.25966 =
      0.27260 0.21460 0.06591 0.09302
C17 1 -0.279454 0.068929 0.831734 11.00000 0.16870
0.22600 =
      0.23050 0.04521 -0.02416 0.12102
AFIX 137
H17A 2 -0.303700 0.016975 0.863523 11.00000 -1.50000
H17B 2 -0.337291 0.084096 0.821471 11.00000 -1.50000
H17C 2 -0.214800 0.136371 0.843430 11.00000 -1.50000
AFIX 0
C18 1 -0.330389 -0.072245 0.748225 11.00000 0.16870
0.22600 =
      0.23050 0.04521 -0.02416 0.12102
AFIX 137
H18A 2 -0.292810 -0.086806 0.717294 11.00000 -1.50000
H18B 2 -0.385438 -0.058096 0.731774 11.00000 -1.50000
H18C 2 -0.365368 -0.135305 0.773713 11.00000 -1.50000
AFIX 6

O10 7 -0.501063 0.000000 0.666667 10.50000 0.06376
0.11078 =
      0.06350 0.01555 0.00777 0.05539
H10A 2 -0.547970 0.003267 0.644217 10.50000 -1.50000
H10B 2 -0.518407 -0.016053 0.630530 10.50000 -1.50000
AFIX 0
HKLF 4

REM shelxs86_a.res in P3(2)21
REM R1 = 0.0449 for 5324 Fo > 4sig(Fo) and 0.0550 for all 5900
data
REM 313 parameters refined using 36 restraints

END

WGHT 0.0557 6.5147

REM Highest difference peak 1.094, deepest hole -1.599, 1-sigma level
0.124
Q1 1 -0.0006 0.6481 0.7963 11.00000 0.05 -1.60
Q2 1 0.0342 0.7023 0.8161 11.00000 0.05 -1.30
Q3 1 -0.2906 0.6607 0.8016 11.00000 0.05 -1.11
Q4 1 -0.0229 0.6789 0.8161 11.00000 0.05 1.09

```

Q5	1	-0.0428	0.3078	0.9369	11.00000	0.05	1.05
Q6	1	0.0000	0.5951	0.8333	10.50000	0.05	-1.04
Q7	1	-0.2906	0.3711	0.8347	11.00000	0.05	0.99
Q8	1	0.0421	1.0421	0.5000	10.50000	0.05	0.91
Q9	1	-0.2398	0.3821	0.8404	11.00000	0.05	-0.80
Q10	1	-0.0477	0.6141	0.8196	11.00000	0.05	-0.77
Q11	1	-0.3114	0.6189	0.8291	11.00000	0.05	0.74
Q12	1	0.1378	0.6736	0.9578	11.00000	0.05	0.72
Q13	1	-0.2481	0.6879	0.8302	11.00000	0.05	0.71
Q14	1	-0.2842	0.6701	0.8799	11.00000	0.05	-0.67
Q15	1	-0.2797	-0.0287	0.8347	11.00000	0.05	0.66
Q16	1	-0.3143	0.6832	0.8247	11.00000	0.05	0.63
Q17	1	-0.3449	-0.0481	0.8051	11.00000	0.05	0.63
Q18	1	0.0655	1.0590	0.4765	11.00000	0.05	-0.62
Q19	1	0.0000	0.3909	0.8333	10.50000	0.05	-0.62
Q20	1	-0.0330	0.4030	0.8167	11.00000	0.05	-0.60

REM The information below was added by Olex2.

REM

REM R1 = 0.0449 for 5324 Fo > 4sig(Fo) and 0.0550 for all 15725 data

REM n/a parameters refined using n/a restraints

REM Highest difference peak 1.09, deepest hole -1.60

REM Mean Shift 0, Max Shift -0.001.

REM +++ Tabular Listing of Refinement Information +++

REM R1_all = 0.0550

REM R1_gt = 0.0449

REM wR_ref = 0.1179

REM GOOF = 1.022

REM Shift_max = -0.001

REM Shift_mean = 0

REM Reflections_all = 15725

REM Reflections_gt = 5324

REM Parameters = n/a

REM Hole = -1.60

REM Peak = 1.09

REM Flack = n/a

;

_olex2_submission_special_instructions 'No special instructions were received'

loop_

_twin_individual_id

_twin_individual_mass_fraction_refined

1 0.68(2)

2 0.32(2)

loop_

_publCIF_info_cif.paper_type

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