

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_gd

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: cu_gd

Bond precision: C-C = 0.0121 Å Wavelength=0.71073

Cell: a=13.9172(6) b=13.9172(6) c=22.8189(11)
 alpha=90 beta=90 gamma=120
Temperature: 150 K

	Calculated	Reported
Volume	3827.6(4)	3827.6(4)
Space group	P 32 2 1	P 32 2 1
Hall group	P 32 2"	P 32 2"
Moiety formula	C30 H34 Cl2 Cu2 Gd N11 O13, 2(C3 H6 N O), H2 O	C30 H34 Cl2 Cu2 Gd N11 O13, 2(C3 H6 N O), H2 O
Sum formula	C36 H48 Cl2 Cu2 Gd N13 O16	C36 H48 Cl2 Cu2 Gd N13 O16
Mr	1274.12	1274.10
Dx,g cm-3	1.658	1.658
Z	3	3
Mu (mm-1)	2.291	2.291
F000	1917.0	1917.0
F000'	1920.02	
h,k,lmax	18,18,29	18,18,29
Nref	5874[3293]	5850
Tmin,Tmax	0.750,0.795	0.708,0.746
Tmin'	0.735	

Correction method= # Reported T Limits: Tmin=0.708 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.78/1.00 Theta(max)= 27.521

R(reflections)= 0.0472(5288) wR2(reflections)= 0.1282(5850)

S = 1.050 Npar= 272

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for N2 --C2 . 8.8 s.u.

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 0.480

From the CIF: _refine_ls_abs_structure_Flack_su 0.030

PLAT213_ALERT_2_C	Atom O1	has ADP max/min Ratio	3.1	prolat
PLAT215_ALERT_3_C	Disordered O2	has ADP max/min Ratio	3.1	Note
PLAT215_ALERT_3_C	Disordered N1	has ADP max/min Ratio	3.1	Note
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range		5.7	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 1 N	Ueq(max)/Ueq(min) Range		4.8	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 1 O	Ueq(max)/Ueq(min) Range		4.5	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range		6.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference N2	--C3	.	0.18	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			03	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			Gd1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			N2	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of			N7	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O8A		0.117	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O10		0.081	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.01213	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #			1	Note
	C30 H34 Cl2 Cu2 Gd N11 O13				
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L=	0.600		2	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.88A	From Gd1	-1.63	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.90A	From O6	0.57	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 ...			7	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension			3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		2	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	.		0.480	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			6.55	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records			9	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			2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records			5	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O1	--N1_f	.	5.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Gd1	--O3	.	6.3	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
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O8A	72.1	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O8B	59.5	Degree
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected	(Rep/Expd) .	1.25	Ratio
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Gd1	--Cu1 ..	9.04	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Cu1	--Cu1 ..	7.03	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Cu1	--Cu1 ..	10.75	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: Cu1	--Cu1 ..	11.21	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	86	Check
	N1 -O1 -N1	1.555 1.555 6.556	22.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	89	Check
	N1 -O2 -N1	1.555 1.555 6.556	30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	107	Check
	N1 -N1 -O1	6.556 1.555 6.556	24.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	196	Check
	H10A -O10 -H10B	1.555 1.555 1.555	40.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	197	Check
	H10B -O10 -H10A	1.555 1.555 1.555	40.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF	#	198	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) .	2.11	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		50	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	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1	Note

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

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

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_ABSTY02_cu_gd
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_STRVA01_cu_gd
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT213_cu_gd
```

```

;
PROBLEM: Atom O1                has ADP max/min Ratio ..... 3.1 prolat
RESPONSE: ...
;
_vrf_PLAT215_cu_gd
;
PROBLEM: Disordered O2          has ADP max/min Ratio ..... 3.1 Note
RESPONSE: ...
;
_vrf_PLAT220_cu_gd
;
PROBLEM: Non-Solvent Resd 1 C    Ueq(max)/Ueq(min) Range      5.7 Ratio
RESPONSE: ...
;
_vrf_PLAT222_cu_gd
;
PROBLEM: Non-Solv. Resd 1 H      Uiso(max)/Uiso(min) Range    6.1 Ratio
RESPONSE: ...
;
_vrf_PLAT234_cu_gd
;
PROBLEM: Large Hirshfeld Difference N2      --C3      .      0.18 Ang.
RESPONSE: ...
;
_vrf_PLAT241_cu_gd
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of      01 Check
RESPONSE: ...
;
_vrf_PLAT242_cu_gd
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of      Gd1 Check
RESPONSE: ...
;
_vrf_PLAT244_cu_gd
;
PROBLEM: Low 'Solvent' Ueq as Compared to Neighbors of      N7 Check
RESPONSE: ...
;
_vrf_PLAT260_cu_gd
;
PROBLEM: Large Average Ueq of Residue Including      O8A      0.117 Check
RESPONSE: ...
;
_vrf_PLAT342_cu_gd
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01213 Ang.
RESPONSE: ...
;
_vrf_PLAT790_cu_gd
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. #      1 Note
RESPONSE: ...
;
_vrf_PLAT911_cu_gd
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      2 Report
RESPONSE: ...
;
_vrf_PLAT934_cu_gd
;
PROBLEM: Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

```

```

RESPONSE: ...
;
_vrf_PLAT972_cu_gd
;
PROBLEM: Check Calcd Resid. Dens. 0.88A From Gd1 -1.63 eA-3
RESPONSE: ...
;
_vrf_PLAT975_cu_gd
;
PROBLEM: Check Calcd Resid. Dens. 0.90A From O6 0.57 eA-3
RESPONSE: ...
;
_vrf_PLAT978_cu_gd
;
PROBLEM: Number C-C Bonds with Positive Residual Density. 0 Info
RESPONSE: ...
;
# end Validation Reply Form

```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

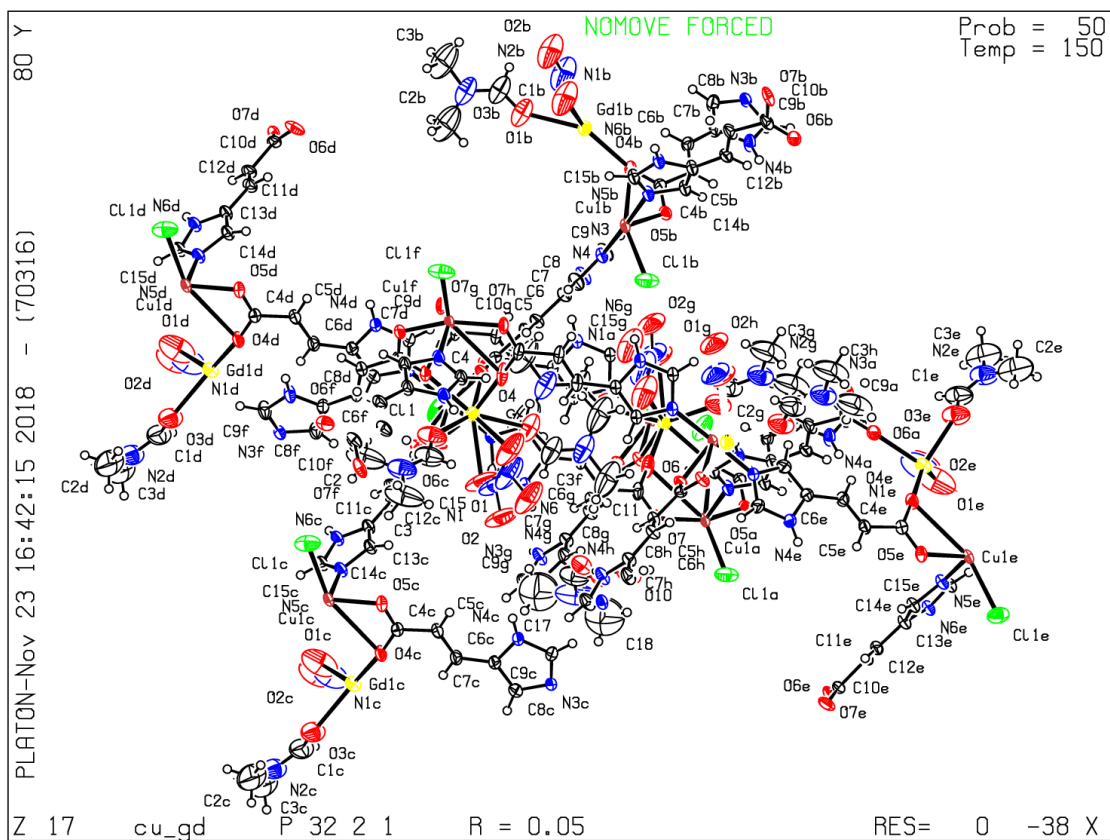
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/10/2018; check.def file version of 15/10/2018



```

data_cu_gd

_audit_update_record
;
2018-11-23 # Formatted by publCIF

;

# publCIF _publ_body_element loop start
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
;
;

;
# publCIF _publ_body_element loop end
_audit_creation_date          2018-11-23

```

```

_audit_creation_method
;
Olex2 1.2
(compiled 2017.03.28 svn.r3405 for OlexSys, GUI svn.r5335)
;
_shelx_SHELXL_version_number      '2014/7'
_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., Giacovazzo, C., Polidori, G., Siliqi, D. & Spagna, R. (2007).
<i>J. Appl. Cryst.</i> 40, 609--613.

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

Sheldrick, G. M. (2015). <i>Acta Cryst.</i> C71, 3--8.
;
_chemical_name_common              ?
_chemical_name_systematic          ?
_chemical_formula_moiety            'C30 H34 Cl2 Cu2 Gd N11 O13, 2(C3 H6 N O), H2 O'
_chemical_formula_sum               'C36 H48 Cl2 Cu2 Gd N13 O16'
_chemical_formula_weight            1274.10
_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'
  'Gd' 'Gd' -0.1653 3.9035
  '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 13.9172(6)
_cell_length_b 13.9172(6)
_cell_length_c 22.8189(11)
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 120
_cell_volume 3827.6(4)
_cell_formula_units_Z 3
_cell_measurement_reflns_used 9899
_cell_measurement_temperature 150(2)
_cell_measurement_theta_max 27.48
_cell_measurement_theta_min 2.46
_shelx_estimated_absorpt_T_max ?
_shelx_estimated_absorpt_T_min ?
_exptl_absorpt_coefficient_mu 2.291
_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 1.658
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?
_exptl_crystal_description prism
_exptl_crystal_F_000 1917
_exptl_crystal_size_max 0.13
_exptl_crystal_size_mid 0.11
_exptl_crystal_size_min 0.1
_exptl_transmission_factor_max 0.7456
_exptl_transmission_factor_min 0.7076
_diffn_reflns_av_R_equivalents 0.0360
_diffn_reflns_av_unetI/netI 0.0659

```

_diffrn_reflns_Laue_measured_fraction_full 0.998
_diffrn_reflns_Laue_measured_fraction_max 0.998
_diffrn_reflns_limit_h_max      18
_diffrn_reflns_limit_h_min     -18
_diffrn_reflns_limit_k_max      18
_diffrn_reflns_limit_k_min     -18
_diffrn_reflns_limit_l_max      29
_diffrn_reflns_limit_l_min      0
_diffrn_reflns_number           11858
_diffrn_reflns_point_group_measured_fraction_full 0.999
_diffrn_reflns_point_group_measured_fraction_max 0.998
_diffrn_reflns_theta_full       25.242
_diffrn_reflns_theta_max        27.521
_diffrn_reflns_theta_min        2.458
_diffrn_ambient_temperature     150(2)
_diffrn_detector_area_resol_mean ?
_diffrn_measured_fraction_theta_full 0.998
_diffrn_measured_fraction_theta_max 0.998
_diffrn_measurement_device_type 'D8 VENTURE Bruker AXS'
_diffrn_measurement_method      'rotation images'
_diffrn_radiation_type          MoK\alpha
_diffrn_radiation_wavelength    0.71073
_diffrn_source                   'Incoatec microfocus sealed tube'
_reflns_Friedel_coverage        0.785
_reflns_Friedel_fraction_full   1.000
_reflns_Friedel_fraction_max    0.999
_reflns_number_gt               5288
_reflns_number_total            5850
_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         1.058
_refine_diff_density_min        -1.704
_refine_diff_density_rms        0.131
_refine_ls_abs_structure_details
;
Refined as an inversion twin.
;

```

```

_refine_ls_abs_structure_Flack      0.48(3)
_refine_ls_extinction_coef          .
_refine_ls_extinction_method        none
_refine_ls_goodness_of_fit_ref      1.050
_refine_ls_hydrogen_treatment       mixed
_refine_ls_matrix_type              full
_refine_ls_number_parameters         272
_refine_ls_number_reflns            5850
_refine_ls_number_restraints         50
_refine_ls_R_factor_all              0.0576
_refine_ls_R_factor_gt              0.0472
_refine_ls_restrained_S_all         1.048
_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^)+(0.0615P)^2^+6.5490P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_weighting_scheme          calc
_refine_ls_wR_factor_gt              0.1206
_refine_ls_wR_factor_ref             0.1282
_refine_special_details
;
  Refined as a 2-component inversion twin.
;
_olex2_refinement_description
;
1. Twinned data refinement
  Scales: 0.52(3)
  0.48(3)
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
  H10B-O10
  0.85 with sigma of 0.02
4. Restrained planarity
  C11, H11, C12, H12
  with sigma of 0.1
  N5, N6, H6, C13, C14, H14, C15, H15
  with sigma of 0.1
5. Uiso/Uanis restraints and constraints
  Uanis(N2) \sim Ueq, Uanis(C1) \sim Ueq, Uanis(O3) \sim Ueq: with sigma
  of
  0.1 and sigma for terminal atoms of 0.2
  Uanis(N1) \sim Ueq, Uanis(O1) \sim Ueq: with sigma of 0.1 and sigma for
  terminal atoms of 0.2
  Uanis(C17) \sim Ueq: with sigma of 0.05 and sigma for terminal atoms of
  0.01
  Uanis(O10) \sim Ueq: with sigma of 0.05 and sigma for terminal atoms of
  0.1

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Uanis(O10) \\sim Ueq, : with sigma of 0.05 and sigma for terminal atoms of 0.01

Uanis(O2) = Uanis(O1)

Uanis(C18) = Uanis(C17)

Uanis(C3) = Uanis(C2)

Uanis(O8B) = Uanis(O8A)

Uanis(C16) = Uanis(C1)

Uanis(C15) = Uanis(N6) = Uanis(C13) = Uanis(C14) = Uanis(N5)

Uanis(N2) = Uanis(C1) = Uanis(O3)

Uanis(O1) = Uanis(N1)

Uanis(N1) = Uanis(O1)

6. Others

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

7.a 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)

7.b Idealised Me refined with everything fixed:

C17(H17A,H17B,H17C), C18(H18A,H18B,H18C)

7.c Idealised Me refined as rotating group:

C2(H2A,H2B,H2C), C3(H3A,H3B,H3C)

;

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_atom_sites_solution_primary direct

_atom_sites_solution_secondary ?

loop_

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_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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_atom_site_disorder_group

Gd1 Gd 0.0000 0.64948(4) 0.8333 0.03035(16) Uani 1 2 d S T P . .

Cu1 Cu -0.29158(9) 0.66732(7) 0.83762(3) 0.0212(2) Uani 1 1 d

C11 C1 -0.4851(2) 0.6410(3) 0.84451(13) 0.0582(8) Uani 1 1 d

O1 O -0.0768(14) 0.4475(9) 0.8593(7) 0.118(5) Uani 1 1 d . U . . .

O2 O -0.033(3) 0.3348(16) 0.8579(11) 0.118(5) Uani 0.5 1 d

O3 O 0.1019(8) 0.6433(9) 0.9172(5) 0.0765(18) Uani 1 1 d . U . . .

O4 O -0.0739(5) 0.7442(5) 0.7847(2) 0.0297(13) Uani 1 1 d

O5 O -0.2264(5) 0.7490(5) 0.7624(2) 0.0262(11) Uani 1 1 d

O6 O -0.5928(6) 0.2553(6) 0.5592(2) 0.0404(17) Uani 1 1 d

O7 O -0.5837(5) 0.1056(5) 0.5813(2) 0.0327(14) Uani 1 1 d

N1 N -0.026(4) 0.428(2) 0.846(2) 0.118(5) Uani 0.5 1 d . U . . .

N2 N 0.1761(10) 0.5946(11) 0.9901(6) 0.0765(18) Uani 1 1 d . U . . .

N3 N 0.1910(5) 0.9687(6) 0.5480(2) 0.0246(13) Uani 1 1 d

N4 N 0.0200(6) 0.9122(7) 0.5756(3) 0.0329(16) Uani 1 1 d
 H4 H -0.0474 0.8987 0.5742 0.040 Uiso 1 1 calc R
 N5 N -0.3497(6) 0.5289(6) 0.7925(2) 0.0275(7) Uani 1 1 d
 N6 N -0.4269(6) 0.3533(6) 0.7687(2) 0.0275(7) Uani 1 1 d
 H6 H -0.4507 0.2834 0.7718 0.033 Uiso 1 1 calc R
 C1 C 0.1461(12) 0.5969(14) 0.9386(7) 0.0765(18) Uani 1 1 d . U
 H1 H 0.1607 0.5548 0.9123 0.092 Uiso 1 1 calc R
 C2 C 0.1658(17) 0.6611(18) 1.0360(10) 0.126(6) Uani 1 1 d
 H2A H 0.1189 0.6134 1.0666 0.189 Uiso 1 1 calc GR
 H2B H 0.1338 0.7026 1.0200 0.189 Uiso 1 1 calc GR
 H2C H 0.2378 0.7114 1.0517 0.189 Uiso 1 1 calc GR
 C3 C 0.2190(17) 0.5246(18) 1.0081(10) 0.126(6) Uani 1 1 d
 H3A H 0.1791 0.4827 1.0419 0.189 Uiso 1 1 calc GR
 H3B H 0.2962 0.5695 1.0176 0.189 Uiso 1 1 calc GR
 H3C H 0.2103 0.4747 0.9768 0.189 Uiso 1 1 calc GR
 C4 C -0.1312(7) 0.7648(7) 0.7501(3) 0.0217(13) Uani 1 1 d
 C5 C -0.0859(7) 0.8121(7) 0.6913(3) 0.0262(15) Uani 1 1 d
 H5 H -0.1300 0.8242 0.6652 0.031 Uiso 1 1 calc R
 C6 C 0.0151(7) 0.8372(7) 0.6752(3) 0.0273(16) Uani 1 1 d
 H6A H 0.0558 0.8215 0.7020 0.033 Uiso 1 1 calc R
 C7 C 0.0689(7) 0.8864(7) 0.6206(3) 0.0267(15) Uani 1 1 d
 C8 C 0.1748(7) 0.9219(8) 0.6026(3) 0.0339(19) Uani 1 1 d
 H8 H 0.2281 0.9155 0.6242 0.041 Uiso 1 1 calc R
 C9 C 0.0991(7) 0.9633(9) 0.5334(4) 0.036(2) Uani 1 1 d
 H9 H 0.0880 0.9909 0.4985 0.043 Uiso 1 1 calc R
 C10 C -0.5671(7) 0.2013(8) 0.5929(3) 0.0295(16) Uani 1 1 d
 C11 C -0.5120(7) 0.2509(8) 0.6502(3) 0.0317(19) Uani 1 1 d
 H11 H -0.4989 0.2077 0.6766 0.038 Uiso 1 1 calc R
 C12 C -0.4817(7) 0.3541(7) 0.6642(3) 0.0293(17) Uani 1 1 d
 H12 H -0.4926 0.3963 0.6363 0.035 Uiso 1 1 calc R
 C13 C -0.4331(7) 0.4070(7) 0.7191(3) 0.0275(7) Uani 1 1 d
 C14 C -0.3841(7) 0.5165(7) 0.7348(3) 0.0275(7) Uani 1 1 d
 H14 H -0.3754 0.5738 0.7104 0.033 Uiso 1 1 calc R
 C15 C -0.3780(7) 0.4279(7) 0.8106(3) 0.0275(7) Uani 1 1 d
 H15 H -0.3651 0.4114 0.8482 0.033 Uiso 1 1 calc R
 O8A O -0.0673(14) 0.1188(15) 0.7673(7) 0.049(3) Uani 0.5 1 d
 O8B O -0.1088(15) 0.0612(16) 0.7439(7) 0.049(3) Uani 0.5 1 d
 N7 N -0.2542(10) 0.0220(14) 0.7804(10) 0.116(7) Uani 1 1 d
 C16 C -0.1490(12) 0.0872(13) 0.7791(7) 0.0765(18) Uani 1 1 d
 C17 C -0.285(4) 0.065(4) 0.8315(17) 0.205(10) Uani 1 1 d . U
 H17A H -0.2802 0.0287 0.8663 0.308 Uiso 1 1 calc
 H17B H -0.3596 0.0504 0.8269 0.308 Uiso 1 1 calc
 H17C H -0.2354 0.1433 0.8347 0.308 Uiso 1 1 calc
 C18 C -0.330(4) -0.076(4) 0.7464(16) 0.205(10) Uani 1 1 d
 H18A H -0.2917 -0.0835 0.7134 0.308 Uiso 1 1 calc
 H18B H -0.3914 -0.0685 0.7329 0.308 Uiso 1 1 calc
 H18C H -0.3576 -0.1410 0.7707 0.308 Uiso 1 1 calc
 O10 O -0.5021(10) 0.0000 0.6667 0.081(4) Uani 1 2 d DS TU P . . .
 H10A H -0.558(4) -0.010(10) 0.647(3) 0.121 Uiso 0.5 1 d DR U
 H10B H -0.53(3) -0.02(3) 0.632(7) 0.121 Uiso 0.5 1 d DR U

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Cu1 0.0305(5) 0.0194(4) 0.0122(3) -0.0002(3) -0.0020(3) 0.0113(4)
C11 0.0372(14) 0.0641(16) 0.0804(17) -0.0375(14) -0.0111(12) 0.0306(12)
O1 0.165(13) 0.036(4) 0.149(10) -0.011(5) -0.079(9) 0.048(6)
O2 0.165(13) 0.036(4) 0.149(10) -0.011(5) -0.079(9) 0.048(6)
O3 0.058(3) 0.072(4) 0.092(4) 0.029(3) -0.014(3) 0.026(3)
O4 0.037(4) 0.037(4) 0.019(2) 0.008(2) 0.002(2) 0.021(3)
O5 0.035(3) 0.027(3) 0.018(2) 0.0050(19) 0.005(2) 0.017(2)
O6 0.040(4) 0.063(5) 0.031(3) -0.025(3) -0.020(3) 0.035(4)
O7 0.028(3) 0.039(3) 0.014(2) -0.007(2) -0.002(2) 0.004(3)
N1 0.165(13) 0.036(4) 0.149(10) -0.011(5) -0.079(9) 0.048(6)
N2 0.058(3) 0.072(4) 0.092(4) 0.029(3) -0.014(3) 0.026(3)
N3 0.022(3) 0.033(4) 0.017(2) 0.000(2) 0.001(2) 0.012(3)
N4 0.024(3) 0.052(5) 0.019(3) 0.009(3) 0.002(3) 0.016(3)
N5 0.0353(19) 0.0274(17) 0.0177(13) -0.0031(12) -0.0043(12) 0.0140(14)
N6 0.0353(19) 0.0274(17) 0.0177(13) -0.0031(12) -0.0043(12) 0.0140(14)
C1 0.058(3) 0.072(4) 0.092(4) 0.029(3) -0.014(3) 0.026(3)
C2 0.087(10) 0.116(12) 0.158(13) 0.078(11) 0.000(9) 0.038(9)
C3 0.087(10) 0.116(12) 0.158(13) 0.078(11) 0.000(9) 0.038(9)
C4 0.028(4) 0.018(3) 0.021(3) 0.001(3) 0.001(3) 0.012(3)
C5 0.032(4) 0.033(4) 0.017(3) 0.001(3) 0.000(3) 0.018(3)
C6 0.031(4) 0.033(4) 0.021(3) 0.007(3) 0.002(3) 0.018(3)
C7 0.025(4) 0.033(4) 0.022(3) 0.005(3) 0.001(3) 0.015(3)
C8 0.028(4) 0.048(5) 0.026(4) 0.005(3) -0.003(3) 0.019(4)
C9 0.024(4) 0.053(6) 0.025(4) 0.011(4) 0.005(3) 0.015(4)
C10 0.022(4) 0.037(5) 0.021(3) -0.012(3) -0.004(3) 0.008(3)
C11 0.028(4) 0.041(5) 0.022(3) -0.014(3) -0.006(3) 0.014(4)
C12 0.030(4) 0.039(5) 0.021(3) -0.010(3) -0.004(3) 0.019(4)
C13 0.0353(19) 0.0274(17) 0.0177(13) -0.0031(12) -0.0043(12) 0.0140(14)
C14 0.0353(19) 0.0274(17) 0.0177(13) -0.0031(12) -0.0043(12) 0.0140(14)
C15 0.0353(19) 0.0274(17) 0.0177(13) -0.0031(12) -0.0043(12) 0.0140(14)
O8A 0.051(8) 0.061(9) 0.049(7) 0.014(5) 0.013(5) 0.040(7)
O8B 0.051(8) 0.061(9) 0.049(7) 0.014(5) 0.013(5) 0.040(7)
N7 0.042(6) 0.095(11) 0.203(18) 0.070(11) -0.013(8) 0.029(7)
C16 0.058(3) 0.072(4) 0.092(4) 0.029(3) -0.014(3) 0.026(3)
C17 0.198(15) 0.213(15) 0.213(15) 0.008(11) -0.014(11) 0.109(12)
C18 0.198(15) 0.213(15) 0.213(15) 0.008(11) -0.014(11) 0.109(12)
O10 0.070(6) 0.113(9) 0.074(7) 0.017(7) 0.008(4) 0.057(5)

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_geom_special_details

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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.

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Gd1 O1 2.528(10) . ?  
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Gd1 O3 2.410(9) 6_556 ?  
Gd1 O4 2.321(5) . ?  
Gd1 O4 2.321(5) 6_556 ?  
Gd1 O6 2.290(6) 3_455 ?  
Gd1 O6 2.290(6) 5_666 ?  
Gd1 N1 2.93(2) . ?  
Gd1 N1 2.93(2) 6_556 ?  
Cu1 Cu1 7.031(2) 6_556 ?  
Cu1 Cu1 10.7509(12) 3_455 ?  
Cu1 Cu1 11.2054(13) 5_666 ?  
Cu1 C11 2.535(3) . ?  
Cu1 O5 2.008(5) . ?  
Cu1 O7 2.051(5) 3_455 ?  
Cu1 N3 1.978(6) 3_465 ?  
Cu1 N5 1.966(7) . ?  
O1 N1 1.65(4) 6_556 ?  
O1 N1 0.93(5) . ?  
O2 O2 1.37(6) 6_556 ?  
O2 N1 1.28(3) . ?  
O2 N1 1.67(4) 6_556 ?  
O3 C1 1.196(17) . ?  
O4 C4 1.252(9) . ?  
O5 C4 1.261(10) . ?  
O6 Gd1 2.290(6) 2_564 ?  
O6 C10 1.248(11) . ?  
O7 Cu1 2.051(5) 2_564 ?  
O7 C10 1.261(11) . ?  
N1 O1 1.65(4) 6_556 ?  
N1 O2 1.67(4) 6_556 ?  
N1 N1 0.86(9) 6_556 ?  
N2 C1 1.252(18) . ?  
N2 C2 1.45(3) . ?  
N2 C3 1.43(2) . ?  
N3 Cu1 1.978(6) 2_674 ?  
N3 C8 1.371(10) . ?  
N3 C9 1.288(11) . ?  
N4 H4 0.8600 . ?  
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N5 C14 1.383(9) . ?  
N5 C15 1.320(11) . ?
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N6 H6 0.8600 . ?
 N6 C13 1.384(9) . ?
 N6 C15 1.321(10) . ?
 C1 H1 0.9300 . ?
 C2 H2A 0.9600 . ?
 C2 H2B 0.9600 . ?
 C2 H2C 0.9600 . ?
 C3 H3A 0.9600 . ?
 C3 H3B 0.9600 . ?
 C3 H3C 0.9600 . ?
 C4 C5 1.489(10) . ?
 C5 H5 0.9300 . ?
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 C9 H9 0.9300 . ?
 C10 C11 1.497(9) . ?
 C11 H11 0.9300 . ?
 C11 C12 1.318(12) . ?
 C12 H12 0.9300 . ?
 C12 C13 1.439(10) . ?
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 C14 H14 0.9300 . ?
 C15 H15 0.9300 . ?
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 O8A C16 1.03(2) . ?
 O8B C16 1.14(2) . ?
 N7 C16 1.280(19) . ?
 N7 C17 1.47(4) . ?
 N7 C18 1.46(4) . ?
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 C17 H17B 0.9600 . ?
 C17 H17C 0.9600 . ?
 C18 H18A 0.9600 . ?
 C18 H18B 0.9600 . ?
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 O10 H10B 0.86(3) . ?
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 O4 Gd1 O3 146.8(3) . . ?
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 O4 Gd1 O3 146.8(3) 6_{-556} 6_{-556} ?
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 O6 Gd1 N1 88.4(10) 5_{-666} 6_{-556} ?
 O6 Gd1 N1 105.1(10) 3_{-455} 6_{-556} ?
 O6 Gd1 N1 88.4(10) 3_{-455} . ?
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 N1 Gd1 Cu1 52.6(9) 6_{-556} 5_{-666} ?
 N1 Gd1 N1 16.9(19) 6_{-556} . ?
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 Cu1 Cu1 Cu1 67.848(9) 6_{-556} 5_{-666} ?
 Cu1 Cu1 Cu1 89.347(12) 3_{-455} 5_{-666} ?

C11 Cu1 Cu1 127.80(6) . 5_666 ?
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 C11 Cu1 Cu1 157.16(7) . 6_556 ?
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 O5 Cu1 C11 106.36(19) . . ?
 O5 Cu1 O7 161.4(3) . 3_455 ?
 O7 Cu1 Cu1 97.84(19) 3_455 6_556 ?
 O7 Cu1 Cu1 25.74(19) 3_455 3_455 ?
 O7 Cu1 Cu1 108.93(17) 3_455 5_666 ?
 O7 Cu1 C11 92.2(2) 3_455 . ?
 N3 Cu1 Cu1 65.9(2) 3_465 6_556 ?
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 N3 Cu1 C11 93.8(2) 3_465 . ?
 N3 Cu1 O5 90.6(2) 3_465 . ?
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 N5 Cu1 C11 90.2(2) . . ?
 N5 Cu1 O5 87.4(2) . . ?
 N5 Cu1 O7 91.1(2) . 3_455 ?
 N5 Cu1 N3 175.9(3) . 3_465 ?
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 N1 O1 Gd1 107(3) . . ?
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 O2 O2 N1 48.4(16) 6_556 6_556 ?
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 N1 O2 N1 30(3) . 6_556 ?
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 C4 O4 Gd1 160.9(6) . . ?
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cu_gd.res created by SHELXL-2014/7


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TITL shelxs86_a.res in P3(2)21
CELL 0.71073 13.9172 13.9172 22.8189 90 90 120
ZERR 3 0.0006 0.0006 0.0011 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 Gd 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 H10b O10
FLAT C11 H11 C12 H12
FLAT N5 N6 H6 C13 C14 H14 C15 H15
ISOR N2 C1 O3
ISOR N1 O1
ISOR 0.05 0.01 C17
ISOR 0.05 0.1 O10
ISOR 0.05 0.01 O10 H10b H10a
EADP O2 O1
EADP C18 C17
EADP C3 C2
EADP O8B O8A
EADP C16 C1
EADP C15 N6 C13 C14 N5
EADP N2 C1 O3
EADP O1 N1
EADP N1 O1

L.S. 100
PLAN 50
HTAB N4 O8A_$4
HTAB N4 O8B_$4
BIND H10b O10
BIND Cu1 Cu1_$1
BIND Cu1 Cu1_$2
BIND Cu1 Cu1_$3
BIND Gd1 Cu1_$1
HTAB
BOND $H
fmap -2
acta
TWIN -1 0 0 0 -1 0 0 0 -1 2
OMIT 0 0 3
REM <olex2.extras>
REM <HklSrc "%.\cu_gd.hkl">
REM </olex2.extras>

WGHT 0.061500 6.549000

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		0.02884	-0.00355	-0.00710	0.01805	
CU1	4	-0.291585	0.667319	0.837621	11.00000	0.03046
0.01936	=					
		0.01221	-0.00017	-0.00202	0.01130	
CL1	3	-0.485093	0.640956	0.844509	11.00000	0.03722
0.06410	=					
		0.08044	-0.03748	-0.01114	0.03063	
O1	7	-0.076813	0.447521	0.859334	11.00000	0.16458
0.03593	=					
		0.14913	-0.01074	-0.07908	0.04768	
O2	7	-0.032864	0.334817	0.857925	10.50000	0.16458
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		0.14913	-0.01074	-0.07908	0.04768	
O3	7	0.101939	0.643313	0.917218	11.00000	0.05762
0.07182	=					
		0.09191	0.02913	-0.01417	0.02615	
O4	7	-0.073862	0.744234	0.784651	11.00000	0.03680
0.03659	=					
		0.01901	0.00752	0.00162	0.02082	
O5	7	-0.226384	0.748998	0.762357	11.00000	0.03524
0.02703	=					
		0.01774	0.00504	0.00504	0.01670	
O6	7	-0.592830	0.255334	0.559169	11.00000	0.04005
0.06297	=					
		0.03132	-0.02523	-0.01953	0.03549	
O7	7	-0.583656	0.105598	0.581342	11.00000	0.02796
0.03884	=					
		0.01430	-0.00719	-0.00165	0.00394	
N1	6	-0.025560	0.428194	0.846488	10.50000	0.16458
0.03593	=					
		0.14913	-0.01074	-0.07908	0.04768	
N2	6	0.176146	0.594626	0.990062	11.00000	0.05762
0.07182	=					
		0.09191	0.02913	-0.01417	0.02615	
N3	6	0.191044	0.968685	0.548033	11.00000	0.02187
0.03265	=					
		0.01654	0.00034	0.00144	0.01164	
N4	6	0.020023	0.912174	0.575558	11.00000	0.02445
0.05155	=					
		0.01941	0.00851	0.00200	0.01647	
AFIX	43					
H4	2	-0.047369	0.898666	0.574237	11.00000	-1.20000
AFIX	0					
N5	6	-0.349699	0.528858	0.792546	11.00000	0.03525
0.02737	=					
		0.01773	-0.00307	-0.00429	0.01402	
N6	6	-0.426858	0.353302	0.768746	11.00000	0.03525
0.02737	=					
		0.01773	-0.00307	-0.00429	0.01402	
AFIX	43					

H6	2	-0.450698	0.283361	0.771846	11.00000	-1.20000
AFIX	0					
C1	1	0.146079	0.596878	0.938615	11.00000	0.05762
0.07182 =						
		0.09191	0.02913	-0.01417	0.02615	
AFIX	43					
H1	2	0.160718	0.554824	0.912262	11.00000	-1.20000
AFIX	0					
C2	1	0.165806	0.661129	1.035960	11.00000	0.08670
0.11566 =						
		0.15836	0.07832	0.00044	0.03821	
AFIX	137					
H2A	2	0.118915	0.613381	1.066567	11.00000	-1.50000
H2B	2	0.133817	0.702626	1.019992	11.00000	-1.50000
H2C	2	0.237849	0.711359	1.051672	11.00000	-1.50000
AFIX	0					
C3	1	0.218967	0.524597	1.008086	11.00000	0.08670
0.11566 =						
		0.15836	0.07832	0.00044	0.03821	
AFIX	137					
H3A	2	0.179082	0.482689	1.041948	11.00000	-1.50000
H3B	2	0.296233	0.569488	1.017562	11.00000	-1.50000
H3C	2	0.210261	0.474716	0.976817	11.00000	-1.50000
AFIX	0					
C4	1	-0.131177	0.764776	0.750105	11.00000	0.02755
0.01823 =						
		0.02076	0.00093	0.00131	0.01246	
C5	1	-0.085866	0.812050	0.691289	11.00000	0.03192
0.03299 =						
		0.01666	0.00073	-0.00027	0.01842	
AFIX	43					
H5	2	-0.129983	0.824190	0.665155	11.00000	-1.20000
AFIX	0					
C6	1	0.015143	0.837200	0.675213	11.00000	0.03066
0.03303 =						
		0.02099	0.00736	0.00199	0.01792	
AFIX	43					
H6A	2	0.055828	0.821516	0.701980	11.00000	-1.20000
AFIX	0					
C7	1	0.068889	0.886379	0.620564	11.00000	0.02510
0.03296 =						
		0.02241	0.00527	0.00094	0.01486	
C8	1	0.174826	0.921930	0.602635	11.00000	0.02816
0.04769 =						
		0.02628	0.00549	-0.00324	0.01930	
AFIX	43					
H8	2	0.228054	0.915465	0.624165	11.00000	-1.20000
AFIX	0					
C9	1	0.099092	0.963311	0.533436	11.00000	0.02431
0.05291 =						
		0.02470	0.01122	0.00544	0.01506	
AFIX	43					
H9	2	0.088017	0.990875	0.498518	11.00000	-1.20000
AFIX	0					

C10	1	-0.567064	0.201281	0.592947	11.00000	0.02158
0.03728 =						
		0.02132	-0.01237	-0.00378	0.00844	
C11	1	-0.512012	0.250884	0.650213	11.00000	0.02758
0.04144 =						
		0.02214	-0.01392	-0.00551	0.01421	
AFIX	43					
H11	2	-0.498895	0.207748	0.676565	11.00000	-1.20000
AFIX	0					
C12	1	-0.481657	0.354101	0.664244	11.00000	0.03003
0.03950 =						
		0.02084	-0.01031	-0.00418	0.01926	
AFIX	43					
H12	2	-0.492586	0.396314	0.636277	11.00000	-1.20000
AFIX	0					
C13	1	-0.433071	0.407038	0.719114	11.00000	0.03525
0.02737 =						
		0.01773	-0.00307	-0.00429	0.01402	
C14	1	-0.384150	0.516461	0.734806	11.00000	0.03525
0.02737 =						
		0.01773	-0.00307	-0.00429	0.01402	
AFIX	43					
H14	2	-0.375409	0.573756	0.710356	11.00000	-1.20000
AFIX	0					
C15	1	-0.377998	0.427934	0.810557	11.00000	0.03525
0.02737 =						
		0.01773	-0.00307	-0.00429	0.01402	
AFIX	43					
H15	2	-0.365069	0.411364	0.848200	11.00000	-1.20000
AFIX	0					
O8A	7	-0.067316	0.118812	0.767336	10.50000	0.05135
0.06129 =						
		0.04915	0.01445	0.01324	0.03968	
O8B	7	-0.108768	0.061183	0.743854	10.50000	0.05135
0.06129 =						
		0.04915	0.01445	0.01324	0.03968	
N7	6	-0.254246	0.021985	0.780388	11.00000	0.04185
0.09498 =						
		0.20320	0.07003	-0.01327	0.02889	
C16	1	-0.149037	0.087189	0.779142	11.00000	0.05762
0.07182 =						
		0.09191	0.02913	-0.01417	0.02615	
C17	1	-0.285038	0.064799	0.831475	11.00000	0.19847
0.21307 =						
		0.21262	0.00839	-0.01408	0.10879	
AFIX	131					
H17A	2	-0.280211	0.028671	0.866273	11.00000	-1.50000
H17B	2	-0.359644	0.050435	0.826858	11.00000	-1.50000
H17C	2	-0.235403	0.143302	0.834718	11.00000	-1.50000
AFIX	0					
C18	1	-0.330285	-0.076211	0.746409	11.00000	0.19847
0.21307 =						
		0.21262	0.00839	-0.01408	0.10879	

AFIX 131
H18A 2 -0.291717 -0.083491 0.713357 11.00000 -1.50000
H18B 2 -0.391440 -0.068532 0.732913 11.00000 -1.50000
H18C 2 -0.357569 -0.141013 0.770671 11.00000 -1.50000
AFIX 0

O10 7 -0.502060 0.000000 0.666667 10.50000 0.06967
0.11328 =
0.07448 0.01675 0.00837 0.05664
H10A 2 -0.558268 -0.010042 0.647048 10.50000 -1.50000
H10B 2 -0.528554 -0.017256 0.631763 10.50000 -1.50000
HKLF 4

REM shelxs86_a.res in P3(2)21
REM R1 = 0.0472 for 5288 Fo > 4sig(Fo) and 0.0576 for all 5850
data
REM 272 parameters refined using 50 restraints

END

WGHT 0.0615 6.5491

REM Instructions for potential hydrogen bonds

HTAB N4 O8A_\$4
HTAB N4 O8B_\$4
EQIV \$5 -x-1, -x+y-1, -z+5/3
HTAB N6 C11_\$5
HTAB C1 O1_\$2
HTAB C1 N1_\$2
HTAB C5 O8A_\$4
HTAB C5 O8B_\$4
HTAB C6 O6_\$1
HTAB C17 C11_\$5
HTAB C18 O10
HTAB O10 O7

REM Highest difference peak 1.058, deepest hole -1.704, 1-sigma level
0.131

Q1	1	0.0316	0.6959	0.8128	11.00000	0.05	-1.70
Q2	1	-0.0389	0.3079	0.9349	11.00000	0.05	1.06
Q3	1	0.0000	0.5997	0.8333	10.50000	0.05	-1.03
Q4	1	-0.1699	0.0284	0.7479	11.00000	0.05	1.02
Q5	1	-0.0399	0.6207	0.8111	11.00000	0.05	-1.01
Q6	1	0.1401	0.6670	0.9605	11.00000	0.05	0.96
Q7	1	-0.2923	0.3733	0.8344	11.00000	0.05	0.88
Q8	1	-0.0064	0.9936	0.5000	10.50000	0.05	-0.85
Q9	1	0.0000	0.7015	0.8333	10.50000	0.05	0.77
Q10	1	0.0393	1.0393	0.5000	10.50000	0.05	0.71
Q11	1	-0.3016	0.6485	0.8044	11.00000	0.05	-0.68
Q12	1	-0.3402	0.3599	0.8306	11.00000	0.05	-0.63
Q13	1	0.2196	0.6356	1.0480	11.00000	0.05	0.63
Q14	1	-0.0360	0.7099	0.8162	11.00000	0.05	-0.62
Q15	1	-0.6500	0.2567	0.5776	11.00000	0.05	0.61
Q16	1	-0.2478	0.3791	0.8461	11.00000	0.05	-0.60

Q17	1	-0.3032	0.3268	0.8180	11.00000	0.05	-0.58
Q18	1	0.2006	0.5193	0.9557	11.00000	0.05	0.57
Q19	1	-0.2705	0.7059	0.8138	11.00000	0.05	-0.56
Q20	1	0.0005	0.3775	0.8505	11.00000	0.05	-0.56
Q21	1	-0.0352	0.4074	0.8206	11.00000	0.05	-0.55
Q22	1	-0.2558	0.6454	0.8255	11.00000	0.05	-0.54
Q23	1	-0.0302	0.1315	0.8212	11.00000	0.05	-0.54
Q24	1	-0.3506	0.6190	0.8211	11.00000	0.05	-0.54
Q25	1	-0.4540	-0.2247	0.7738	11.00000	0.05	-0.53
Q26	1	-0.3552	-0.0431	0.8061	11.00000	0.05	0.53
Q27	1	-0.3175	0.6198	0.8636	11.00000	0.05	-0.53
Q28	1	-0.0701	0.5608	0.8162	11.00000	0.05	0.52
Q29	1	0.0845	1.0517	0.4832	11.00000	0.05	-0.51
Q30	1	0.1903	0.5104	0.9223	11.00000	0.05	0.50
Q31	1	-0.0432	0.3459	0.8282	11.00000	0.05	0.49
Q32	1	-0.0600	0.9105	0.5072	11.00000	0.05	-0.49
Q33	1	0.0403	1.0391	0.4727	11.00000	0.05	-0.49
Q34	1	0.1627	0.6812	1.0622	11.00000	0.05	-0.48
Q35	1	-0.3553	-0.0298	0.9376	11.00000	0.05	0.48
Q36	1	0.0692	0.7219	0.9206	11.00000	0.05	0.47
Q37	1	-0.1415	0.3601	0.9091	11.00000	0.05	0.46
Q38	1	0.0094	0.3764	0.8779	11.00000	0.05	0.46
Q39	1	0.1010	0.6783	0.9406	11.00000	0.05	-0.46
Q40	1	-0.4097	-0.0374	0.8327	11.00000	0.05	0.46
Q41	1	-0.4174	0.3708	0.8274	11.00000	0.05	-0.46
Q42	1	-0.0962	0.7250	0.7470	11.00000	0.05	0.45
Q43	1	-0.2940	0.3569	0.8641	11.00000	0.05	-0.45
Q44	1	-0.3900	-0.1889	0.7477	11.00000	0.05	0.45
Q45	1	-0.4954	0.6754	0.8140	11.00000	0.05	-0.45
Q46	1	0.2345	0.4879	1.0216	11.00000	0.05	-0.45
Q47	1	-0.2902	0.0496	0.7982	11.00000	0.05	-0.43
Q48	1	-0.3880	0.3640	0.7444	11.00000	0.05	0.43
Q49	1	-0.2795	-0.0240	0.8368	11.00000	0.05	0.43
Q50	1	-0.0496	0.7308	0.8411	11.00000	0.05	0.42

REM The information below was added by Olex2.

REM

REM R1 = 0.0472 for 5288 Fo > 4sig(Fo) and 0.0576 for all 11877 data

REM n/a parameters refined using n/a restraints

REM Highest difference peak 1.06, deepest hole -1.70

REM Mean Shift 0, Max Shift -0.001.

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

REM R1_all = 0.0576

REM R1_gt = 0.0472

REM wR_ref = 0.1282

REM GOOF = 1.050

REM Shift_max = -0.001

REM Shift_mean = 0

REM Reflections_all = 11877

REM Reflections_gt = 5288

REM Parameters = n/a

REM Hole = -1.70

REM Peak = 1.06

REM Flack = n/a

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