

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 2a

Bond precision:	C-C = 0.0126 Å	Wavelength=0.71073
Cell:	a=19.1968 (4)	b=27.0713 (5) c=25.2042 (4)
	alpha=90	beta=92.012 (2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	13090.1 (4)	13090.1 (4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C270 H168 Gd8 N2 O52 [+ solvent]	?
Sum formula	C270 H168 Gd8 N2 O52 [+ solvent]	C270 H184 Gd8 N2 O55
Mr	5530.08	5594.12
Dx, g cm ⁻³	1.403	1.417
Z	2	2
Mu (mm ⁻¹)	2.068	2.069
F000	5460.0	5524.0
F000'	5459.59	
h, k, lmax	22, 32, 29	22, 32, 29
Nref	23040	23027
Tmin, Tmax	0.615, 0.813	0.531, 1.000
Tmin'	0.433	

Correction method= # Reported T Limits: Tmin=0.531 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 24.999

R(reflections)= 0.0460(17981)

wR2(reflections)=
0.1376(23027)

S = 1.024

Npar= 1495

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

PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O19	--H19A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O21	--H21A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O26	--H26A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O26	--H26B	.	Please Check



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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.77	Report
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	09	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	010	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	023	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Gd2	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01259	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C31 - C32	1.53	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H10 ..H26A	1.93	Ang.
	1-x,1-y,2-z =	3_667	Check



Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C270 H184 Gd8 N2 O55

Atom count from the _atom_site data: C270 H168 Gd8 N2 O52

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_sum C270 H184 Gd8 N2 O55

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	540.00	540.00	0.00
H	368.00	336.00	32.00
Gd	16.00	16.00	0.00
N	4.00	4.00	0.00
O	110.00	104.00	6.00

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	135	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	55.88	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report

PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C32 -C45	0.17	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C63 -C68	0.16	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C93 -C98	0.15	Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C8	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C8_a .	1.63	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C7 - C8 .	1.50	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C8 - C9 .	1.52	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd1 (III) .	3.10	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd2 (III) .	3.25	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd3 (III) .	3.35	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd4 (III) .	3.26	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3540	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.5	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree

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

7 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
 4 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 6 ALERT type 5 Informative message, check

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.

