

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: 2

Bond precision:	C-C = 0.0173 A	Wavelength=0.71073
Cell:	a=19.1149 (3)	b=26.8237 (5) c=24.8999 (4)
	alpha=90	beta=91.480 (2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	12762.7 (4)	12762.7 (4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C135 H85 Gd4 N O26 [+ solvent]	?
Sum formula	C135 H85 Gd4 N O26 [+ solvent]	C135 H95 Gd4 N O29
Mr	2766.05	2824.08
Dx, g cm ⁻³	1.440	1.468
Z	4	4
Mu (mm ⁻¹)	2.121	2.124
F000	5464.0	5584.0
F000'	5463.59	
h, k, lmax	22, 31, 29	22, 31, 29
Nref	22520	22504
Tmin, Tmax	0.607, 0.809	0.323, 1.000
Tmin'	0.423	

Correction method= # Reported T Limits: Tmin=0.323 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 25.010

R(reflections)= 0.0583(16560)

wR2(reflections)=
0.1657(22504)

S = 1.001

Npar= 1479

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

PLAT213_ALERT_2_B	Atom C95	has ADP max/min Ratio		4.2	prolat
PLAT220_ALERT_2_B	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	6.2	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C1	--C2	.	8.0 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C3	--C8	.	8.9 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C12	--C13	.	7.2 s.u.
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C13	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C95	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C103	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C3	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C7	Check
PLAT245_ALERT_2_B	U(iso) H26A	Smaller than U(eq)	O26 by	0.069	Ang**2
PLAT420_ALERT_2_B	D-H Bond Without	Acceptor	O17 --H17A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without	Acceptor	O18 --H18A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without	Acceptor	O26 --H26A	.	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		2.21	Report	
PLAT213_ALERT_2_C	Atom C97	has ADP max/min Ratio		3.5 prolat	
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	10.0 Ratio	
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C2	--C3	.	5.8 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C13	--C14	.	7.0 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O18	--C91	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	--C4	.	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C6	--C7	.	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C7	--C8	.	0.23 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C8	--C9	.	0.24 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C9	--C10	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C10	--C15	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C38	--C39	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C80	--C81	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C92	--C105	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C107	--C108	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C107	--C120	.	0.17 Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O7	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O18	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O19	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O22	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O23	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C4	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C6	Check

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C8	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C11	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C15	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C97	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C101	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C117	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C129	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C131	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	Gd2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C93	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C94	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C104	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds		0.0173	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C1 - C2	.	1.53	Ang.
PLAT415_ALERT_2_C	Short	Inter D-H...H-X H18A ..H97	.	2.14	Ang.
		1-x,-y,-z =		3_655	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: C135 H95 Gd4 N1 O29
 Atom count from the _atom_site data: C135 H85 Gd4 N1 O26

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 4
 From the CIF: _chemical_formula_sum C135 H95 Gd4 N O29
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	540.00	540.00	0.00
H	380.00	340.00	40.00
Gd	16.00	16.00	0.00
N	4.00	4.00	0.00
O	116.00	104.00	12.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 31 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 16 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 100.91 Why ?
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 12 Report
 PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
 PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
 PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0400 Report
 PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0200 Report
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C92 -C105 . 1.42 Ang.
 PLAT432_ALERT_2_G Short Inter X...Y Contact C67 ..C69 . 3.18 Ang.
 1-x,1-y,-z = 3_655 Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Gd1 (III) . 3.31 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Gd2 (III) . 3.19 Info

PLAT794_ALERT_5_G	Tentative Bond Valency for Gd3	(III)	.	3.29	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd4	(III)	.	3.41	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			141	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			4.9	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
14 **ALERT level B** = A potentially serious problem, consider carefully
43 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
28 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
49 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
17 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.

