

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: Compound_1

Bond precision: C-C = 0.0038 A

Wavelength=0.71073

Cell: a=13.1921(7) b=9.9012(4) c=20.9851(11)
 alpha=90 beta=95.176(2) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	2729.9(2)	2729.8(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety	C10 H24 Gd N4	
formula	O10, 3(Cl O4), 2(H2 O)	C10H24GdN4O10,3(ClO4),2(H2O)
Sum formula	C10 H28 Cl3 Gd N4 O24	C10 H28 Cl3 Gd N4 O24
Mr	851.96	851.96
Dx,g cm-3	2.073	2.073
Z	4	4
Mu (mm-1)	2.832	2.832
F000	1692.0	1692.0
F000'	1694.16	
h,k,lmax	18,14,29	18,14,29
Nref	8328	8285
Tmin,Tmax	0.672,0.868	0.440,0.710
Tmin'	0.376	

Correction method= # Reported T Limits: Tmin=0.440 Tmax=0.710
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 30.514

R(reflections)= 0.0280(7543)

wR2(reflections)= 0.0733(8285)

S = 1.081

Npar= 433

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 G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.27	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	16	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact O11 ..C2	2.96	Ang.
	1-x,1-y,1-z =	3_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C2	3.11	Ang.
	-x,1-y,1-z =	3_566	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	19	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd1 (III) .	3.34	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	24	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

