

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vv3gd

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: vv3gd

Bond precision: C-C = 0.0046 Å Wavelength=0.71073

Cell: a=11.493(2) b=26.991(5) c=6.0220(12)
 alpha=90 beta=118.65(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1639.4(7)	1639.4(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C15 H13 Gd O11	C15 H13 Gd O11
Sum formula	C15 H13 Gd O11	C15 H13 Gd O11
Mr	526.50	526.50
Dx, g cm ⁻³	2.133	2.133
Z	4	4
Mu (mm ⁻¹)	4.108	4.108
F000	1020.0	1020.0
F000'	1019.92	
h, k, lmax	13, 32, 7	13, 31, 7
Nref	1450	1386
Tmin, Tmax	0.681, 0.782	
Tmin'	0.657	

Correction method= Not given

Data completeness= 0.956 Theta(max)= 25.025

R(reflections)= 0.0156(1382)

wR2(reflections)=
0.0410(1386)

S = 1.095

Npar= 143

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

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.955 Why?

Author Response: Data collection was performed using only phi scans with MX1 Synchrotron, which led to relatively low data completeness.



Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.15 Do !
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.69 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 63 Report



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.23 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c 12/a Note
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 14% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O3 . 106.5 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O6 . 108.3 Degree
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 7 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1 (III) . 3.30 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 18 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 98% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

24 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

5 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
4 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

