

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) trytri

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: trytri

Bond precision: C-C = 0.0058 A

Wavelength=0.71073

Cell: a=11.0671 (2) b=15.9865 (3) c=16.2163 (3)
 alpha=106.0779 (9) beta=95.5905 (10) gamma=95.9480 (9)
Temperature: 299 K

	Calculated	Reported
Volume	2718.02 (9)	2718.01 (9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 Gd N8 O6, C15 H11 Gd N7 O12, 2(C2 H3 N)	C30 H22 Gd N8 O6, C15 H11 Gd N7 O12, 2(C2 H3 N)
Sum formula	C49 H39 Gd2 N17 O18	C49 H39 Gd2 N17 O18
Mr	1468.47	1468.47
Dx, g cm ⁻³	1.794	1.794
Z	2	2
Mu (mm ⁻¹)	2.510	2.510
F000	1448.0	1448.0
F000'	1447.92	
h,k,lmax	16,23,24	16,23,24
Nref	18964	18544
Tmin,Tmax	0.667,0.747	0.688,0.746
Tmin'	0.593	

Correction method= # Reported T Limits: Tmin=0.688 Tmax=0.746
AbsCorr = NUMERICAL

Data completeness= 0.978

Theta(max)= 32.048

R(reflections)= 0.0430 (13179)

wR2(reflections)=
0.0890 (18544)

S = 1.011

Npar= 777

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

PLAT913_ALERT_3_B Missing # of Very Strong Reflections in FCF 118 Note
5 0 0, 1 1 0, 5 2 0, -2 3 0, -1 3 0, 0 4 0,
1 4 0, -3 5 0, 0 5 0, 2 5 0, -2 6 0, -1 7 0,
0 7 0, 1 8 0, 2 -8 1, -2 -7 1, 3 -7 1, -1 -6 1,
0 -6 1, -1 -4 1, 2 -4 1, -4 -3 1, 0 -2 1, -3 -1 1,

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for O14 --N12 . 5.5 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O8 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O10 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 N14 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N17 0.106 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.444 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
1 0 0, 0 1 0, 0 -1 1, 0 0 1, 0 1 1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 256 Report
3 0 0, 5 0 0, -4 1 0, 1 1 0, 2 1 0, 4 1 0,
-2 2 0, 5 2 0, -2 3 0, -1 3 0, 0 4 0, 1 4 0,
3 4 0, -6 5 0, -3 5 0, 0 5 0, 2 5 0, -2 6 0,
-1 7 0, 0 7 0, 1 8 0, 2 -8 1, -2 -7 1, 3 -7 1,
-1 -6 1, 0 -6 1, -4 -5 1, -2 -5 1, 4 -5 1, -3 -4 1,
-1 -4 1, 1 -4 1, 2 -4 1, -4 -3 1, -1 -3 1, 2 -3 1,
4 -3 1, -3 -2 1, -1 -2 1, 0 -2 1, 1 -2 1, 5 -2 1,
-4 -1 1, -3 -1 1, -2 -1 1, 1 -1 1, 2 -1 1, -5 0 1,
-3 0 1, -2 0 1, 1 0 1, 2 0 1, 3 0 1, -1 1 1,
1 1 1, 4 1 1, -2 2 1, 0 2 1, 1 2 1, 3 2 1,
-2 3 1, -2 4 1, -1 5 1, 0 5 1, -4 6 1, 1 6 1,
-3 7 1, 0 -8 2, -2 -7 2, 1 -7 2, -1 -6 2, 2 -6 2,
-4 -5 2, 3 -5 2, 4 -5 2, -3 -4 2, -1 -3 2, -5 -2 2,
-2 -2 2, -1 -2 2, 0 -2 2, 1 -2 2, 3 -2 2, -1 -1 2,
2 -1 2, 4 -1 2, -4 0 2, -1 0 2, 0 0 2, 1 0 2,
5 0 2, 0 1 2, 1 1 2, 4 1 2, -5 2 2, 3 2 2,
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Gd1 1.10 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From O11 . -0.51 eA-3

Alert level G

PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0 0.996 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd1 --O3 . 7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd1 --O4 . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd1 --O5 . 8.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd2 --O8 . 16.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd2 --O15 . 8.8 s.u.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note

C15 H11 Gd N7 O12

PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	159	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.2	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		1.233	Note
	Predicted wR2: Based on SigI**2	7.22 or SHELX Weight	8.80	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		4	Info

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

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

