

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gdmnt_0m

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: gdmnt_0m

Bond precision:	C-C = 0.0092 A	Wavelength=0.71073	
Cell:	a=13.6798 (7)	b=18.3572 (9)	c=17.5889 (10)
	alpha=90	beta=92.146 (2)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	4413.9 (4)	4413.9 (4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H18 Gd N14 Na5 S8	C28 H18 Gd N14 Na5 S8
Sum formula	C28 H18 Gd N14 Na5 S8	C28 H18 Gd N14 Na5 S8
Mr	1079.25	1079.24
Dx, g cm ⁻³	1.624	1.624
Z	4	4
Mu (mm ⁻¹)	1.970	1.970
F000	2124.0	2124.0
F000'	2128.18	
h, k, l _{max}	17, 22, 21	17, 22, 21
Nref	9019	8914
Tmin, Tmax	0.681, 0.821	0.462, 0.746
Tmin'	0.668	

```
Correction method= # Reported T Limits: Tmin=0.462 Tmax=0.746
AbsCorr = MULTI-SCAN
```

Data completeness= 0.988 Theta (max)= 26.372

```
R(reflections)= 0.0439( 7675)      wR2(reflections)=
S = 1.023                        0.1199( 8914)
Npar= 511
```

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

PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	8.3 Ratio
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	Na5 Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C01G Check	

Alert level C

PLAT220_ALERT_2_C	NonSolvent	Resd 1	N	Ueq(max)/Ueq(min) Range	3.4 Ratio	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N014 Check		
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N4 Check		
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N01A Check		
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N01B Check		
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N01D Check		
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N7 Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Na2 Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Na3 Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Na4 Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C019 Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C01F Check		
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C01H Check		
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00917 Ang.		
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			9 Note		
	1 1 0,	0 2 0,	-1 0 1,	1 0 1,	-1 1 1,	0 1 1,
	1 1 1,	0 2 1,	0 0 2,			
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		19 Report		
	0 17 13,	1 17 13,	1 16 14,	1 15 15,	2 15 15,	1 13 16,
	0 14 16,	1 14 16,	0 12 17,	1 12 17,	2 12 17,	3 12 17,
	-1 13 17,	0 13 17,	0 10 18,	1 10 18,	0 11 18,	-7 0 19,
	2 8 19,					
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang From Gd01		2.07 eA-3		
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.94Ang From Gd01		2.06 eA-3		
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.77Ang From Gd01		-1.92 eA-3		
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.82Ang From Gd01		-1.61 eA-3		
PLAT977_ALERT_2_C	Check Negative Difference Density on H01E	.		-0.33 eA-3		

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	17.38 Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4 Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	33 Note
	Gd01 N000 N00Y C012 N014 C017 H01A H01B	
	H01C C018 C019 N01A N01B C01C H01D H01E	
	H01F N01D C01E H01G H01H H01I C01F C01G	
	C01H C01I H01J H01K H01L C01J H01M H01N	
	H01O	
PLAT774_ALERT_1_G	Check X-Y Bond in CIF: Na3 --Na2 ..	4.22 Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Gd01 (III) .	3.34 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4 Note

PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	77	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		3	Note
	1 0 1, 0 2 0, -1 1 1,			
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.584	Note
	Predicted wR2: Based on SigI**2	4.64 or SHELX Weight	11.72	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
21 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 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
3 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT220_gdmnt_0m
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range           8.3 Ratio
RESPONSE: ...
;
_vrf_PLAT242_gdmnt_0m
;
PROBLEM: Low         'MainMol' Ueq as Compared to Neighbors of      Na5 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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.

