

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gitam035

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: gitam035

Bond precision: C-C = 0.0130 A Wavelength=1.54180

Cell: a=9.3610(4) b=8.3498(3) c=16.7159(8)
 alpha=90 beta=106.310(5) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1253.98(10)	1253.98(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	?
Moiety formula	C7 H3 N2 O8 Sm, O	?
Sum formula	C7 H3 N2 O9 Sm	C7 H3 N2 O9 Sm
Mr	409.47	409.46
Dx,g cm-3	2.169	2.169
Z	4	4
Mu (mm-1)	35.635	35.635
F000	772.0	772.0
F000'	754.73	
h,k,lmax	11,10,20	11,10,20
Nref	2474	2436
Tmin,Tmax	0.000,0.001	0.030,0.050
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.030 Tmax=0.050
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 72.000

R(reflections)= 0.0543(2405) wR2(reflections)= 0.1656(2436)

S = 1.176 Npar= 172

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 A

PLAT211_ALERT_2_A ADP of Atom C6 is N.P.D. or (nearly) 2D ... Please Check
PLAT971_ALERT_2_A Check Calcd Residual Density 1.32A From 0101 4.03 eA-3

Alert level B

SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10
Absolute value of the parameter shift to su ratio given 0.104
Additional refinement cycles may be required.
PLAT430_ALERT_2_B Short Inter D...A Contact 05 .. 0102 .. 2.78 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact 07 .. 0101 .. 2.76 Ang.
PLAT971_ALERT_2_B Check Calcd Residual Density 0.75A From Sml 2.54 eA-3

Alert level C

PLAT080_ALERT_2_C Maximum Shift/Error 0.10 Why ?
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1
PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio 3.6 prolat
PLAT220_ALERT_2_C Large Non-Solvent 0 Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0130 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact 05 .. 0101 .. 2.85 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT971_ALERT_2_C Check Calcd Residual Density 0.71A From Sml 2.22 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.85A From Sml 1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.80A From Sml -2.45 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.75A From Sml -2.29 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.24A From Sml -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.35A From Sml -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.45A From Sml -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.30A From 01 -1.52 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.86A From 05 1.17 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 1.04A From N1 1.10 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.76A From 03 1.07 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.88A From 0101 0.96 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.98A From 06 0.94 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.91A From 01 0.79 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.60A From 0102 0.77 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.97A From 0101 0.75 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.52A From 08 -1.35 eA-3

Alert level G

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 3 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 15.23 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/n P21/c Note
PLAT302_ALERT_4_G Anion/Solvent Disorder Percentage = 100 Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 0101 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 0102 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 79 Do !
06 -SM1 -N2 -08 -168.00 15.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 80 Do !
03 -SM1 -N2 -08 -94.00 15.00 1.455 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 81 Do !
01 -SM1 -N2 -08 -86.00 15.00 2.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 82 Do !
02 -SM1 -N2 -08 -20.00 15.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 83 Do !

O4	-SM1 -N2 -O8	119.00 15.00	3.675	1.555	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4	Linear Torsion Angle ...	#	84	Do !		
O5	-SM1 -N2 -O8	104.00 15.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4	Linear Torsion Angle ...	#	85	Do !		
O7	-SM1 -N2 -O8	16.00 14.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4	Linear Torsion Angle ...	#	86	Do !		
N1	-SM1 -N2 -O8	43.00 15.00	1.555	1.555	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4	Linear Torsion Angle ...	#	87	Do !		
O6	-SM1 -N2 -O8	-166.00 15.00	3.575	1.555	1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4	Linear Torsion Angle ...	#	88	Do !		
SM1	-SM1 -N2 -O8	-168.00 15.00	3.575	1.555	1.555	1.555	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.		1.29	Ratio		
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: SM1 -- SM1 ..			4.03	Ang.		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			24	Note		
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL			2014	Note		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600			36	Note		
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities				Please Check		

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
32 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
15 ALERT type 4 Improvement, methodology, query or suggestion
3 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*, 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 21/04/2015; check.def file version of 09/03/2015

Datablock gitam035 - ellipsoid plot

