

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lpg\_a

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: lpg\_a**

Bond precision:	C-C = 0.0094 Å	Wavelength=0.71073
Cell:	a=10.419(8) alpha=90	b=29.386(16) beta=101.33(3) c=15.691(10) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	4711(5)	4711(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	8(C19 H30 O3 S), C6 H14	8(C19 H30 O3 S), C6 H14
Sum formula	C158 H254 O24 S8	C158 H254 O24 S8
Mr	2794.09	2794.08
Dx, g cm-3	0.985	0.985
Z	1	1
Mu (mm-1)	0.149	0.149
F000	1522.0	1522.0
F000'	1523.62	
h,k,lmax	12,35,19	12,35,19
Nref	8947	8917
Tmin,Tmax	0.968,0.988	0.573,0.747
Tmin'	0.901	

Correction method= # Reported T Limits: Tmin=0.573 Tmax=0.747  
AbsCorr = MULTI SCAN

Data completeness= 0.997                      Theta (max)= 25.682

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R(reflections)= 0.1158( 5979)      wR2(reflections)=
S = 1.151                        0.2965( 8917)
Npar= 512
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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.

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### Alert level B

PLAT049\_ALERT\_1\_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9849 Check

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### Alert level C

PLAT082\_ALERT\_2\_C High R1 Value ..... 0.12 Report  
PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.02 Report  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio  
PLAT220\_ALERT\_2\_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 4.8 Ratio  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C15 --C16 . 6.1 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C15 --C19 . 5.2 s.u.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C34 --C38 . 0.20 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C34 --C38A . 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C37 --C38 . 0.16 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C26 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including C1S 0.162 Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00939 Ang.  
PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check  
PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note  
C19 H30 O3 S  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 24.630 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.378 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.104 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 25 Report  
1 2 0, 1 3 0, 2 3 0, 1 7 0, -1 0 1, -1 2 1,  
0 3 1, -1 4 1, 0 4 1, -2 0 2, 0 0 2, -1 1 2,  
0 1 2, -1 3 2, 0 3 2, -1 0 3, -1 2 3, 0 2 3,  
-1 3 3, 0 0 4, -1 1 4, 7 19 6, 9 1 10, -7 11 13,  
-3 2 15,  
PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 8 Note  
0 2 0, 1 2 0, 1 3 0, 2 3 0, -2 0 2, 0 1 2,  
0 2 3, 0 0 4,  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check  
-1 4 4,

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### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 20 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H-Atoms 19 Report  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
H5 H6 H2 H3  
PLAT063\_ALERT\_4\_G Crystal Size Possibly too Large for Beam Size .. 0.70 mm

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	10.00	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		6	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		7	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par		0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar		0.0020	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar		0.0200	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffraction_ambient_temperature .....	(K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6S	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SC	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SA	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SB	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SC	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1)	17%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H18B ..H37C		1.71	Ang.
	1/2+x, 3/2-y, -1/2+z =		4_675	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H31A ..H38C		1.87	Ang.
	x, y, z =		1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		14	Note
	H1SA H1SB H1SC H2SA H2SB H3SA H3SB H4SA			
	H4SB H5SA H5SB H6SA H6SB H6SC			
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...		0.01	Ang.
	C37A -H37D 1_555 1_555 .....	#	117	Check
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...		0.01	Ang.
	C5S -H5SA 1_555 1_555 .....	#	134	Check
PLAT721_ALERT_1_G	Bond Calc 0.97000, Rep 0.96000 Dev...		0.01	Ang.
	C6S -H6SC 1_555 1_555 .....	#	139	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C19 H30 O3 S			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C6 H14			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		139	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please	Do !
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta (Min) [Deg]=		2.11	Note
	0 2 0, 0 1 1, 0 2 1,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		16	Note
	-1 0 3, -1 1 2, -1 1 4, -1 2 1, -1 2 3, -1 3 2,			
	-1 3 3, -1 4 1, 0 0 2, 0 2 1, 0 3 1, 0 3 2,			

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      0 4 1, 1 2 0, 1 7 0, 2 3 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 5.010 Note
      Predicted wR2: Based on SigI**2 5.92 or SHELX Weight 25.77
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 ALERT type 2 Indicator that the structure model may be wrong or deficient
16 ALERT type 3 Indicator that the structure quality may be low
35 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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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.

